

Patent Claims

- 1. A ligand-binding domain (LBD) of the ultraspiracle protein (USP) in crystalline form.
- A LBD according to Claim 1, wherein the LBD is a LBD of the Heliothis virescens USP.
- A LBD according to Claim 1, wherein the LBD comprises the amino acid
 sequence as shown in SEQ ID NO: 1.
 - 4. A LBD according to Claim 1, wherein the LBD exists in the form of a complex with a ligand.
- 15 5. A LBD according to Claim 1, wherein the LBD has the structure coordinates defined in Table 1, below:

Table 1

REMARK coordinates from restrained individual B-factor refinement

0 REMARK refinement resolution: 20.0 - 1.65 A

REMARK starting r= 0.2151 free_r= 0.2506

REMARK final r= 0.2112 free_r= 0.2459

REMARK B rmsd for bonded mainchain atoms= 1.437 target= 1.5

REMARK B rmsd for bonded sidechain atoms= 2.272 target= 2.0 REMARK B rmsd for angle mainchain atoms= 2.299 target= 2.0

REMARK B rmsd for angle sidechain atoms= 2.235 target= 2.5

REMARK rweight= 0.1000 (with wa= 1.12122)

REMARK target= mlf steps= 30

REMARK sg= P4(3)22 a= 58.211 b= 58.211 c= 144.687 alpha= 90 beta= 90 gamma= 90

REMARK parameter file 1 : CNS_TOPPAR:protein_rep.param

REMARK parameter file 2 : CNS_TOPPAR:water_rep.param

REMARK parameter file 3 : eph.par

REMARK molecular structure file: alternate.mtf

REMARK input coordinates: anneal_2.pdb

35 REMARK reflection file= /home/billas/USP/SCALE0400/merge1A65/usp_20a1a65 10 cv REMARK ncs= none

REMARK B-correction resolution: 6.0 - 1.65

REMARK initial B-factor correction applied to fobs :

REMARK B11= -1.985 B22= -1.985 B33= 3.970

40 REMARK B12= 0.000 B13= 0.000 B23= 0.000

REMARK B-factor correction applied to coordinate array B: -0.193

REMARK bulk solvent: density level= 0.33501 e/A³, B-factor= 48.7849 A²

REMARK reflections with |Fobs|/sigma_F < 0.0 rejected

REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected

45 REMARK theoretical total number of refl. in resol. range: 30842 (100.0 %)

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REMARK number of unobserved reflections (no entry or |F|=0): 1417 ( 4.6 %)
                                                    0(0.0%)
     REMARK number of reflections rejected:
                                                   29425 ( 95.4 % )
     REMARK total number of reflections used:
     REMARK number of reflections in working set:
                                                   26453 (85.8 %)
                                                   2972 ( 9.6 % )
     REMARK number of reflections in test set:
5
     CRYST1 58.211 58.211 144.687 90.00 90.00 90.00 P 43 2 2
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     REMARK DATE: 4-Jun-00 14:33:10
                                     created by user: billas
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             4 N ALA 203
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49 CA ILE 210

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	ATOM	72 NH1 ARG 212	17.055 23.527 46.148 1.00 43.03
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	ATOM	106 CE MET 216	14.187 23.383 52.223 1.00 30.33
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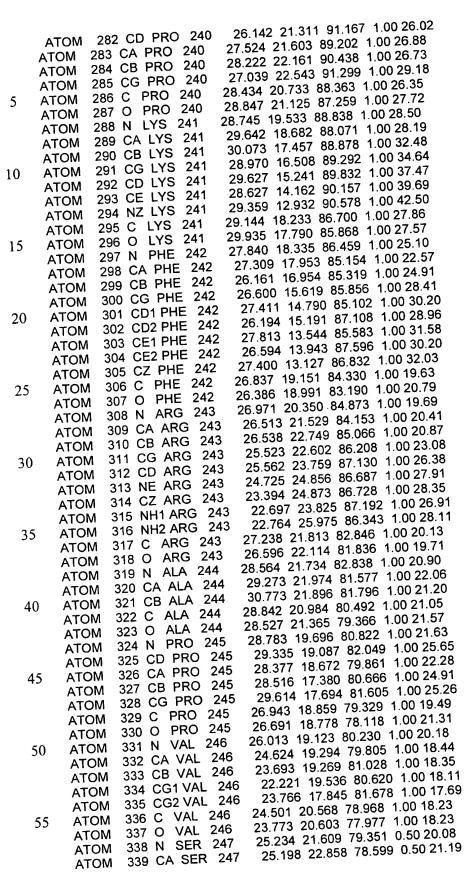
ATOM 108 O MET 216 18.955 20.998 52.755 1.00 32.43 109 N GLU 217 **ATOM** 18.381 18.982 51.923 1.00 34.02 **ATOM** 110 CA GLU 217 18.908 18.212 53.046 1.00 35.35 111 CB GLU 217 18.470 16.745 52.919 1.00 33.44 **ATOM** 5 **ATOM** 112 CG GLU 217 18.729 15.871 54.148 1.00 32.91 **ATOM** 113 CD GLU 217 17.999 16.372 55.389 1.00 32.03 114 OE1 GLU 217 115 OE2 GLU 217 ATOM 17.001 17.104 55.242 1.00 33.02 18.419 16.032 56.511 1.00 34.58 MOTA 116 C GLU 217 MOTA 20.421 18.293 53.105 1.00 37.01 117 O GLU 217 10 MOTA 21.006 18.276 54.190 1.00 37.08 118 N SER 218 21.036 18.406 51.928 1.00 39.66 MOTA 119 CA SER 218 ATOM 22.491 18.476 51.795 1.00 42.68 120 CB SER 218 22.913 18.001 50.408 1.00 43.25 ATOM 121 OG SER 218 22.571 16.640 50.214 1.00 46.19 ATOM 122 C SER 218 15 23.083 19.856 52.027 1.00 44.17 MOTA **ATOM** 123 O SER 218 24.250 19.978 52.395 1.00 43.66 **ATOM** 124 N LEU 219 22.291 20.895 51.797 1.00 46.04 125 CA LEU 219 **ATOM** 22.773 22.254 51.982 1.00 48.34 **ATOM** 126 CB LEU 219 21.706 23.265 51.556 1.00 49.36 20 127 CG LEU 219 21.670 23.631 50.072 1.00 50.71 **ATOM** 128 CD1 LEU 219 ATOM 21.879 22.395 49.219 1.00 51.07 129 CD2 LEU 219 20.341 24.307 49.760 1.00 51.61 MOTA 130 C LEU 219 23.183 22.530 53.416 1.00 49.65 ATOM 131 O LEU 219 132 N VAL 220 133 CA VAL 220 134 CB VAL 220 22.501 22.140 54.363 1.00 49.02 ATOM 25 24.318 23.205 53.552 1.00 51.55 **ATOM** ATOM 24.868 23.592 54.843 1.00 53.29 26.250 22.945 55.085 1.00 52.35 MOTA 135 CG1 VAL 220 136 CG2 VAL 220 ATOM 26.774 23.341 56.456 1.00 51.60 26.142 21.426 54.965 1.00 50.84 ATOM 30 137 C VAL 220 25.030 25.106 54.770 1.00 55.56 MOTA 138 O VAL 220 25.929 25.613 54.097 1.00 56.16 ATOM ATOM 139 N ALA 221 24.147 25.823 55.450 1.00 57.83 MOTA 140 CA ALA 221 24.190 27.278 55.428 1.00 60.51 141 CB ALA 221 MOTA 22.782 27.845 55.601 1.00 60.73 142 C ALA 221 35 **ATOM** 25.108 27.838 56.499 1.00 61.87 143 O ALA 221 **ATOM** 25.475 27.143 57.452 1.00 62.13 **ATOM** 144 N ALA 222 25.490 29.100 56.326 1.00 62.85 **ATOM** 145 CA ALA 222 26.345 29.756 57.295 1.00 63.37 146 CB ALA 222 26.612 31.196 56.871 1.00 63.59 **MOTA** 147 C ALA 222 40 **ATOM** 25.564 29.719 58.601 1.00 63.51 **MOTA** 148 O ALA 222 24.422 30.176 58.659 1.00 63.95 **ATOM** 149 N ALA 223 26.173 29.150 59.636 1.00 63.63 MOTA 150 CA ALA 223 25.532 29.044 60.939 1.00 63.10 151 CB ALA 223 152 C ALA 223 **ATOM** 26.558 28.627 61.984 1.00 63.64 45 **ATOM** 24.874 30.365 61.339 1.00 62.58 153 O ALA 223 154 N ALA 224 **ATOM** 25.557 31.333 61.678 1.00 63.33 MOTA 23.544 30.399 61.290 1.00 61.31 **ATOM** 155 CA ALA 224 22.789 31.599 61.644 1.00 59.25 156 CB ALA 224 MOTA 21.323 31.440 61.220 1.00 58.51 157 C ALA 224 50 MOTA 22.878 31.880 63.143 1.00 58.07 158 O ALA 224 22.988 30.943 63.939 1.00 58.18 MOTA 159 N GLU 225 22.844 33.159 63.528 1.00 56.07 **ATOM** 160 CA GLU 225 **ATOM** 22.909 33.507 64.950 1.00 54.05 161 CB GLU 225 22.498 34.969 65.221 1.00 54.53 MOTA 55 162 CG GLU 225 22.700 35.401 66.703 1.00 55.83 **ATOM** 21.439 35.872 67.407 1.00 56.62 **ATOM** 163 CD GLU 225 **ATOM** 164 OE1 GLU 225 21.407 35.822 68.663 1.00 57.35 165 OE2 GLU 225 20.464 36.314 66.743 1.00 57.42 **ATOM**



21.901 32.594 65.611 1.00 52.71 ATOM 166 C GLU 225 20.737 32.557 65.201 1.00 52.66 MOTA 167 O GLU 225 22.334 31.840 66.612 1.00 50.26 **MOTA** 168 N GLU 226 21.391 30.960 67.256 1.00 47.92 169 CA GLU 226 **ATOM** 170 CB GLU 226 21.858 29.513 67.196 1.00 49.61 MOTA 171 CG GLU 226 20.778 28.525 67.641 1.00 49.78 MOTA 19.333 28.959 67.359 1.00 51.91 172 CD GLU 226 MOTA 18.452 28.312 67.956 1.00 50.08 173 OE1 GLU 226 **MOTA** 174 OE2 GLU 226 19.039 29.909 66.543 1.00 51.77 **ATOM** 175 C GLU 226 21.015 31.344 68.670 1.00 46.28 10 ATOM 176 O GLU 226 21.839 31.794 69.476 1.00 47.17 MOTA 177 N PHE 227 19.733 31.155 68.942 1.00 41.52 MOTA 19.138 31.503 70.206 1.00 38.73 178 CA PHE 227 MOTA 17.723 32.022 69.963 1.00 40.03 179 CB PHE 227 **ATOM** 17.640 33.061 68.876 1.00 40.91 180 CG PHE 227 15 MOTA 181 CD1 PHE 227 17,775 32,703 67,542 1,00 40,72 MOTA 17.464 34.402 69.192 1.00 42.62 182 CD2 PHE 227 ATOM 17.739 33.661 66.535 1.00 42.04 17.426 35.374 68.188 1.00 42.27 183 CE1 PHE 227 ATOM 184 CE2 PHE 227 ATOM 17.564 34.996 66.857 1.00 42.02 185 CZ PHE 227 20 ATOM 186 C PHE 227 19.119 30.339 71.174 1.00 34.83 MOTA 187 O PHE 227 19.218 29.178 70.778 1.00 34.52 **ATOM** 18.982 30.687 72.445 1.00 33.69 **ATOM** 188 N GLN 228 18.979 29.735 73.540 1.00 32.01 189 CA GLN 228 MOTA 19,290 30,468 74,847 1,00 34,80 190 CB GLN 228 **ATOM** 191 CG GLN 228 20.680 31.080 74.935 1.00 39.39 **MOTA** 21.768 30.029 74.916 1.00 40.63 192 CD GLN 228 **ATOM** 22.117 29.504 73.860 1.00 44.27 22.301 29.706 76.093 1.00 42.65 193 OE1 GLN 228 **MOTA** 194 NE2 GLN 228 MOTA 17.678 28.974 73.736 1.00 28.92 195 C GLN 228 30 MOTA 196 O GLN 228 197 N PHE 229 17.035 29.174 74.750 1.00 28.29 MOTA 17.283 28.120 72.794 1.00 28.04 MOTA 198 CA PHE 229 16.056 27.340 72.996 1.00 25.30 MOTA 15.767 26.411 71.821 1.00 27.02 199 CB PHE 229 **ATOM** 15.066 27.055 70.680 1.00 28.71 200 CG PHE 229 35 ATOM 15.599 28.170 70.052 1.00 28.96 201 CD1 PHE 229 MOTA 13.903 26.480 70.173 1.00 30.61 202 CD2 PHE 229 MOTA 14.991 28.708 68.918 1.00 29.32 203 CE1 PHE 229 MOTA 13.284 26.998 69.046 1.00 31.44 13.829 28.117 68.412 1.00 31.43 204 CE2 PHE 229 MOTA 205 CZ PHE 229 40 MOTA ATOM 206 C PHE 229 ATOM 207 O PHE 229 ATOM 208 N LEU 230 ATOM 209 CA LEU 230 16.276 26.434 74.195 1.00 23.81 15.385 26.202 75.014 1.00 22.15 17.487 25.899 74.263 1.00 20.44 17.848 24.964 75.302 1.00 21.42 18.255 23.631 74.650 1.00 20.34 17.191 22.855 73.834 1.00 22.70 ATOM 210 CB LEU 230 45 ATOM 211 CG LEU 230 17.860 21.762 73.013 1.00 23.14 16.130 22.252 74.773 1.00 21.55 ATOM 212 CD1 LEU 230 ATOM 213 CD2 LEU 230 ATOM 214 C LEU 230 19.017 25.540 76.094 1.00 20.71 19.977 26.038 75.524 1.00 20.61 ATOM 215 O LEU 230 50 18.931 25.467 77.411 1.00 20.48 ATOM 216 N ARG 231 20.018 25.997 78.211 1.00 20.62 20.023 27.525 78.176 1.00 20.50 ATOM 217 CA ARG 231 ATOM 218 CB ARG 231 ATOM 219 CG ARG 231 ATOM 220 CD ARG 231 18.907 28.184 79.017 1.00 24.52 17.560 28.025 78.342 1.00 27.62 55 ATOM 221 NE ARG 231 ATOM 222 CZ ARG 231 16.465 28.674 79.060 1.00 28.14 15.846 28.165 80.118 1.00 28.35 ATOM 223 NH1 ARG 231 16.208 26.986 80.598 1.00 27.27



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	ATOM 340 05 05 15 05 404 24 202 8() 517 0.50 25.07 715
	ATOM 341 OG SER 247 25.464 24.252 77.189 0.50 21.32 AC1 25.712 22.621 77.189 0.50 21.32 AC1 25.180 23.161 76.217 0.50 21.62 AC1 25.180 23.161 76.217 0.50 21.62
	ATOM 343 O SER 247 25.180 23.101 77.076 1.00 20.43
5	AIUW 544 1 5 64 000 01 500 /5 /50 1.00 21.02
	A LOW 340 07. 0 - 00 EAA 30 EDA 75 910 1.00 24.01
	ATOM 347 OG SER 248 29.660 21.330 74.003 1.00 22.36
	ATOM 348 C SER 248 26.271 20.000 73.697 1.00 22.32
10	ATOM 343 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9
	A 1 O W 330 W 223 2 462 10 185 74 791 1.00 22.20
	ATOM 352 CB LEU 249 23.904 16.040 75.054 1.00 25.52
	ATOM 333 00 22 - 34 444 16 010 76 922 1.00 20.33
15	ATUM 334 OD 1220 - 05 200 16 3/1 7/16/43 1.00 27.01
	ATOM 356 C LEU 249 23.358 20.152 74.352 1.00 21.05
	A (U V) 337 3 2 2 3 3 3 3 1 10 7 7 5 7 1 7 1 1 0 2 1 1 0
	A 10 N 330 N 3 04 005 33 008 74 856 1.00 21.22
20	A LOW 309 ON 319 - 204 02 044 76 119 1.00 20.00
	ATOM 361 SG CYS 250 20.853 22.243 73 684 1.00 22.49
	ATOM 302 0 010 200 04 607 23 302 /2.828 1.00 23.00
2.5	A LUIVI 303 0 0 0 0 0 0 0 70E 22 220 73 hbh 1.00 22.01
25	ATOM 365 CA GLN 251 24.313 24.064 72.317 1.00 26.13
	A LOW 300 OB 02.1 = 1.00 31.00 1.00 31.00
	ATOM 307 00 01.1 1
30	ATOM 369 OE1 GLN 251 28.146 26.020 /3.846 1.00 36.70
30	ATOM 370 NE2 GLN 251 27.520 23.270 71.255 1.00 23.96
	ATUN 371 0 0=1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
	A LOW 5/2 5 5 5 5 6 6 04 008 /1 3/3 1.00 25/17
35	ATOM 374 CA ILE 252 24.475 21.140 70.493 1.00 25.71
5.	A 1 UNI 373 33 12 04 20E 10 727 64 419 1.00 23.12
	ATUN 370 000 40 EOR /11 han 1.00 20.11
	ATOM 378 CD1 ILE 252 26.874 18.3 69 642 1.00 25.30
4	0 ATOM 379 C ILE 252 23.032 21.103 08.448 1.00 25.88
	ATOM 500 0 '
	ATOM 382 CA GLY 253 20.698 21.167 70.213 1.00 24.98
	ATOM 383 C GLY 253 20.327 22.437 68.561 1.00 24.56
4	15 A O VI 304 O O C
	ATOM 386 CA ASN 254 20.483 24.929 69.642 1.00 24.10
	ATOM 387 CB ASN 254 21.003 25.333 75.884 1.00 24.90
	A I DIVI 300 00 7.0.
•	50 ATOM 390 ND2 ASN 254 21.020 26.511 72.934 1.00 25.59
	ATOM 391 C ASN 254 20.990 25.172 67.418 1.00 25.49
	A 1 UNI 332 3 7 3 1 3 67 67 915 1.00 27 01
	ATOM 394 CA LYS 255 22.718 24.669 66.572 1.00 29.40
	ATOM 395 CB LYS 255 24.121 24.001 67 112 1.00 33.68
	ATOM 390 00 255 26 481 24.293 67.392 1.00 34.00
	ATOM 397 CD LYS 255 26.481 24.293 07.332 113





	ATOM		27.280 24.027 66.150 1.00 35.57
	MOTA	399 NZ LYS 255	28.719 23.853 66.527 1.00 33.75
	MOTA		21.816 23.924 65.608 1.00 26.04
_	MOTA	401 O LYS 255	21.539 24.415 64.507 1.00 25.57
5	MOTA	402 N GLN 256	21.358 22.741 66.009 1.00 24.02
	MOTA	403 CA GLN 256	20.498 21.967 65.121 1.00 23.89
	ATOM	404 CB GLN 256	20.325 20.546 65.658 1.00 25.47
	ATOM	405 CG GLN 256	21.676 19.880 65.887 1.00 28.63
10	ATOM	406 CD GLN 256	21.565 18.517 66.534 1.00 30.93
10	ATOM	407 OE1 GLN 256	20.710 18.301 67.387 1.00 32.63
	ATOM	408 NE2 GLN 256	22.439 17.599 66.149 1.00 30.18
	ATOM	409 C GLN 256	19.156 22.658 64.915 1.00 24.45
	ATOM	410 O GLN 256	18.596 22.598 63.828 1.00 24.20
1.0	ATOM		18.662 23.338 65.942 1.00 23.21
15	ATOM		17.390 24.059 65.816 1.00 22.41
	ATOM		16.895 24.535 67.180 1.00 20.26
	ATOM	414 CG2 ILE 257	15.636 25.401 67.021 1.00 21.15
	ATOM	415 CG1 ILE 257	16.607 23.298 68.039 1.00 22.12
20	ATOM	416 CD1 ILE 257	16.309 23.620 69.517 1.00 21.36
20	ATOM		17.558 25.253 64.877 1.00 23.91
	ATOM		16.677 25.544 64.060 1.00 21.49
	ATOM	419 N ALA 258	18.684 25.949 64.994 1.00 23.86
	ATOM	420 CA ALA 258	18.939 27.081 64.103 1.00 25.37 20.313 27.705 64.416 1.00 26.26
25	ATOM	421 CB ALA 258	18.906 26.588 62.656 1.00 25.01
25	ATOM	422 C ALA 258	18.306 27.238 61.783 1.00 25.01
	ATOM	423 O ALA 258	19.555 25.450 62.403 1.00 23.72
	MOTA	424 N ALA 259 425 CA ALA 259	19.602 24.865 61.063 1.00 24.51
	MOTA	426 CB ALA 259	20.442 23.613 61.058 1.00 24.62
30	ATOM		18.187 24.525 60.623 1.00 24.36
30	ATOM ATOM	427 C ALA 259 428 O ALA 259	17.846 24.693 59.464 1.00 23.27
	ATOM	429 N LEU 260	17.374 24.015 61.544 1.00 23.02
	ATOM	430 CA LEU 260	15.986 23.685 61.188 1.00 24.75
	ATOM	430 CA LEU 200 431 CB LEU 260	15.237 23.070 62.366 1.00 26.22
35	ATOM	431 CB LEU 260	15.550 21.633 62.742 1.00 31.27
33	ATOM	432 CG LEU 260 433 CD1 LEU 260	14.906 21.342 64.082 1.00 32.20
	ATOM	434 CD2 LEU 260	15.054 20.679 61.658 1.00 33.32
	ATOM	435 C LEU 260	15.214 24.902 60.750 1.00 25.40
	ATOM	436 O LEU 260	14.391 24.821 59.834 1.00 23.40
40	ATOM	437 N VAL 261	15.439 26.031 61.419 1.00 25.21
70	ATOM	438 CA VAL 261	14.735 27.247 61.055 1.00 26.95
	ATOM	439 CB VAL 261	15.050 28.411 62.036 1.00 25.46
	ATOM	440 CG1 VAL 261	14.386 29.700 61.544 1.00 27.40
	ATOM	441 CG2 VAL 261	14.520 28.075 63.434 1.00 27.42
45	ATOM	442 C VAL 261	15.104 27.671 59.640 1.00 26.53
	ATOM	443 O VAL 261	14.232 28.035 58.850 1.00 25.34
	ATOM	444 N VAL 262	16.396 27.611 59.320 1.00 27.29
	ATOM	445 CA VAL 262	16.874 27.995 57.993 1.00 28.11
	ATOM	446 CB VAL 262	18.430 27.910 57.905 1.00 30.08
50	ATOM	447 CG1 VAL 262	18.883 27.872 56.441 1.00 33.75
-	ATOM	448 CG2 VAL 262	19.051 29.104 58.606 1.00 32.97
	ATOM	449 C VAL 262	16.267 27.075 56.939 1.00 26.73
	ATOM	450 O VAL 262	15.909 27.511 55.840 1.00 26.28
	ATOM	451 N TRP 263	16.177 25.794 57.286 1.00 24.38
55	MOTA	452 CA TRP 263	15.623 24.775 56.402 1.00 25.26
	ATOM	453 CB TRP 263	15.831 23.406 57.052 1.00 23.10
	MOTA	454 CG TRP 263	15.102 22.286 56.409 1.00 24.27
	MOTA	455 CD2 TRP 263	13,881 21.697 56.873 1.00 24.86



13,536 20.681 55.962 1.00 25.93 ATOM 456 CE2 TRP 263 13.051 21.936 57.974 1.00 24.53 457 CE3 TRP 263 MOTA 15.441 21.624 55.267 1.00 24.80 458 CD1 TRP 263 MOTA 14.501 20.655 54.990 1.00 27.16 459 NE1 TRP 263 ATOM 12.391 19.895 56.115 1.00 26.26 460 CZ2 TRP 263 MOTA 11.911 21.151 58.132 1.00 23.32 461 CZ3 TRP 263 MOTA 11.598 20.144 57.204 1.00 23.73 462 CH2 TRP 263 MOTA 14.125 25.047 56.175 1.00 24.66 463 C TRP 263 MOTA 13.645 25.081 55.037 1.00 25.81 464 O TRP 263 MOTA 13.391 25.278 57.252 1.00 24.56 465 N ALA 264 ATOM 10 11.949 25.506 57.103 1.00 25.04 466 CA ALA 264 ATOM 11.304 25.733 58.464 1.00 26.00 467 CB ALA 264 MOTA 11.675 26.701 56.205 1.00 27.22 468 C ALA 264 MOTA 10.838 26.640 55.293 1.00 24.71 469 O ALA 264 ATOM 12.372 27.794 56.489 1.00 28.16 470 N ARG 265 15 MOTA 12.227 29.024 55.724 1.00 32.11 471 CA ARG 265 MOTA 13.250 30.066 56.218 1.00 33.47 472 CB ARG 265 MOTA 13.155 31.408 55.520 1.00 36.25 ATOM 473 CG ARG 265 14.169 32.397 56.078 1.00 39.06 ATOM 474 CD ARG 265 15.545 31.972 55.823 1.00 42.06 475 NE ARG 265 20 ATOM 16.609 32.534 56.391 1.00 43.94 476 CZ ARG 265 MOTA 16.447 33.541 57.244 1.00 44.49 477 NH1 ARG 265 MOTA 17.827 32.092 56.110 1.00 43.52 478 NH2 ARG 265 MOTA 12.424 28.767 54.225 1.00 32.76 479 C ARG 265 **ATOM** 11.843 29.460 53.392 1.00 35.61 480 O ARG 265 **ATOM** 25 13.227 27.771 53.872 1.00 33.71 481 N ASP 266 MOTA 13.465 27.492 52.466 1.00 34.17 482 CA ASP 266 MOTA 14.931 27.106 52.236 1.00 37.32 483 CB ASP 266 MOTA 15.879 28.293 52.374 1.00 40.62 484 CG ASP 266 MOTA 15.556 29.392 51.866 1.00 40.66 485 OD1 ASP 266 **ATOM** 30 16.959 28.128 52.985 1.00 43.94 486 OD2 ASP 266 MOTA 12.544 26.447 51.833 1.00 33.93 487 C ASP 266 MOTA 12.664 26.156 50.646 1.00 32.38 488 O ASP 266 MOTA 11.640 25.869 52.619 1.00 32.18 489 N ILE 267 **ATOM** 10.694 24.897 52.077 1.00 30.21 490 CA ILE 267 MOTA 35 9.820 24.279 53.210 1.00 29.16 491 CB ILE 267 ATOM 8.586 23.588 52.620 1.00 31.21 492 CG2 ILE 267 ATOM 10.643 23.291 54.038 1.00 29.01 493 CG1 ILE 267 **ATOM** 11.069 22.051 53.278 1.00 28.89 494 CD1 ILE 267 MOTA 9.800 25.670 51.093 1.00 30.06 495 C ILE 267 40 MOTA 9.256 26.715 51.421 1.00 29.41 496 O ILE 267 MOTA 9.653 25.164 49.862 1.00 31.41 497 N PRO 268 **ATOM** 10.216 23.921 49.300 1.00 31.06 498 CD PRO 268 MOTA 8.813 25.857 48.879 1.00 31.62 499 CA PRO 268 **MOTA** 8.686 24.830 47.755 1.00 31.63 500 CB PRO 268 **MOTA** 45 10.012 24.126 47.811 1.00 34.16 501 CG PRO 268 MOTA 7,459 26.286 49.444 1.00 31.83 502 C PRO 268 MOTA 6.762 25.483 50.051 1.00 31.61 503 O PRO 268 MOTA 7.128 27.566 49.267 1.00 31.08 504 N HIS 269 MOTA 5.867 28.164 49.715 1.00 31.47 505 CA HIS 269 MOTA 50 4.677 27.277 49.300 1.00 33.82 506 CB HIS 269 MOTA 4.710 26.845 47.865 1.00 36.44 507 CG HIS 269 MOTA 4.694 25.611 47.305 1.00 37.13 508 CD2 HIS 269 MOTA 4.734 27.740 46.816 1.00 39.48 509 ND1 HIS 269 MOTA 4.731 27.078 45.672 1.00 37.91 510 CE1 HIS 269 MOTA 55 4.706 25.785 45.941 1.00 39.31 511 NE2 HIS 269 MOTA 5.745 28.465 51.210 1.00 30.01 ATOM 512 C HIS 269 4.796 29.133 51.638 1.00 28.74 ATOM 513 O HIS 269



5	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	514 N PHE 270 515 CA PHE 270 516 CB PHE 270 517 CG PHE 270 518 CD1 PHE 270 519 CD2 PHE 270 520 CE1 PHE 270 521 CE2 PHE 270	6.693 27.994 52.012 1.00 28.26 6.607 28.222 53.454 1.00 27.87 7.728 27.468 54.178 1.00 26.66 7.661 27.563 55.684 1.00 24.18 6.867 26.683 56.415 1.00 24.15 8.385 28.536 56.372 1.00 26.34 6.792 26.775 57.822 1.00 22.45 8.316 28.637 57.778 1.00 24.45	
10	ATOM ATOM ATOM ATOM ATOM	522 CZ PHE 270 523 C PHE 270 524 O PHE 270 525 N SER 271 526 CA SER 271	7.516 27.754 58.494 1.00 23.03 6.650 29.707 53.811 1.00 28.65 5.866 30.175 54.634 1.00 29.19 7.558 30.448 53.184 0.50 29.83 7.676 31.876 53.463 0.50 31.34	AC1 AC1
15	ATOM ATOM ATOM ATOM ATOM	527 CB SER 271 528 OG SER 271 529 C SER 271 530 O SER 271 531 N GLN 272	8.959 32.432 52.839 0.50 31.74 10.104 31.869 53.460 0.50 31.64 6.458 32.663 52.974 0.50 32.85 6.301 33.839 53.296 0.50 33.99 5.599 32.009 52.197 1.00 33.79	AC1 AC1 AC1 AC1
20	ATOM ATOM ATOM ATOM	532 CA GLN 272 533 CB GLN 272 534 CG GLN 272 535 CD GLN 272 536 OE1 GLN 272	4.378 32.642 51.696 1.00 35.22 3.910 31.928 50.423 1.00 39.02 4.777 32.210 49.191 1.00 43.59 4.608 31.169 48.086 1.00 45.89 3.488 30.794 47.727 1.00 47.68	
25	ATOM ATOM ATOM ATOM ATOM	537 NE2 GLN 272 538 C GLN 272 539 O GLN 272 540 N LEU 273	5.729 30.703 47.534 1.00 48.15 3.255 32.633 52.742 1.00 35.20 2.288 33.397 52.648 1.00 33.55 3.383 31.756 53.736 1.00 33.18	
30	ATOM ATOM ATOM ATOM ATOM	541 CA LEU 273 542 CB LEU 273 543 CG LEU 273 544 CD1 LEU 273 545 CD2 LEU 273	2.402 31.651 54.811 1.00 31.26 2.695 30.398 55.653 1.00 30.14 2.671 29.015 54.988 1.00 29.04 3.273 27.989 55.930 1.00 28.99 1.231 28.638 54.645 1.00 29.21	
35	ATOM ATOM ATOM ATOM ATOM	546 C LEU 273 547 O LEU 273 548 N GLU 274 549 CA GLU 274 550 CB GLU 274	2.500 32.880 55.722 1.00 30.95 3.556 33.513 55.793 1.00 30.58 1.416 33.208 56.420 1.00 31.28 1.435 34.332 57.355 1.00 32.85 0.154 34.378 58.195 1.00 35.60	
40	ATOM ATOM ATOM ATOM ATOM	551 CG GLU 274 552 CD GLU 274 553 OE1 GLU 274 554 OE2 GLU 274 555 C GLU 274	-1.039 35.022 57.511 1.00 40.50 -0.954 36.543 57.494 1.00 43.35 -1.788 37.171 56.807 1.00 44.88 -0.062 37.109 58.169 1.00 45.29 2.615 34.079 58.287 1.00 32.91	
45	ATOM ATOM ATOM ATOM ATOM	556 O GLU 274 557 N MET 275 558 CA MET 275 559 CB MET 275 560 CG MET 275	2.867 32.936 58.693 1.00 31.56 3.331 35.136 58.632 1.00 31.54 4.483 35.010 59.507 1.00 31.78 5.094 36.392 59.748 1.00 34.73 6.288 36.403 60.673 1.00 37.61	
50	ATOM ATOM ATOM ATOM	561 SD MET 275 562 CE MET 275 563 C MET 275 564 O MET 275	7.574 35.262 60.158 1.00 39.49 7.940 35.869 58.496 1.00 39.54 4.149 34.351 60.838 1.00 31.91 4.885 33.474 61.305 1.00 31.90	
55	ATOM ATOM ATOM ATOM ATOM ATOM ATOM	565 N GLU 276 566 CA GLU 276 567 CB GLU 276 568 CG GLU 276 569 CD GLU 276 570 OE1 GLU 276 571 OE2 GLU 276	3.052 34.764 61.458 1.00 31.07 2.684 34.184 62.736 1.00 30.79 1.499 34.938 63.341 1.00 35.06 1.866 36.382 63.755 1.00 37.66 3.043 36.434 64.731 1.00 40.34 2.978 35.751 65.774 1.00 41.45 4.034 37.157 64.464 1.00 42.59	

	Lea 43 //2-roleign Commission
5	ATOM 572 C GLU 276 2.3 ATOM 573 O GLU 276 2.52 ATOM 574 N ASP 277 1.97 ATOM 575 CA ASP 277 1.7 ATOM 576 CB ASP 277 0.8 ATOM 577 CG ASP 277 -0.6 ATOM 578 OD1 ASP 277 -0.6
10	ATOM 579 OD2 ASP 277 -1. ATOM 580 C ASP 277 3.0 ATOM 581 O ASP 277 3.2 ATOM 582 N GLN 278 4.0 ATOM 583 CA GLN 278 5.0 ATOM 584 CB GLN 278 6.
15	ATOM 585 CG GLN 278 5. ATOM 586 CD GLN 278 6. ATOM 587 OE1 GLN 278 8 ATOM 588 NE2 GLN 278 6
20	ATOM 590 O GLN 278 6.4 ATOM 591 N ILE 279 5.8 ATOM 592 CA ILE 279 6.3 ATOM 593 CB ILE 279 6.3
25	ATOM 595 CG1 ILE 279 6 ATOM 596 CD1 ILE 279 6 ATOM 597 C ILE 279 5.6 ATOM 598 O ILE 279 6.2
30	ATOM 600 CA LEU 280 ATOM 601 CB LEU 280 ATOM 602 CG LEU 280 ATOM 603 CD1 LEU 280
35	ATOM 604 CD2 LEU 280 ATOM 605 C LEU 280 4 ATOM 606 O LEU 280 4 ATOM 607 N LEU 281 4 ATOM 608 CA LEU 281
40	ATOM 612 CD2 LEU 281
4:	ATOM 617 CB ILE 282 ATOM 618 CG2 ILE 282
5	ATOM 619 CG1 ILE 282 ATOM 620 CD1 ILE 282 0 ATOM 621 C ILE 282 ATOM 622 O ILE 282 ATOM 623 N LYS 283
4	ATOM 624 CA LYS 283 ATOM 625 CB LYS 283 ATOM 626 CG LYS 283 ATOM 627 CD LYS 283 ATOM 628 CF LYS 283

ATOM 629 NZ LYS 283

2.388 32.693 62.596 1.00 29.05 .529 31.946 63.559 1.00 28.93 .973 32.250 61.411 1.00 26.93 1.716 30.817 61.223 1.00 24.95 0.817 30.565 60.005 1.00 26.30 0.656 30.768 60.320 1.00 26.04 -0.984 31.102 61.476 1.00 29.19 -1.492 30.596 59.410 1.00 26.42 3.056 30.089 61.069 1.00 25.34 3.226 28.967 61.579 1.00 25.43 4.007 30.721 60.373 1.00 23.47 5.338 30.132 60.203 1.00 23.93 6.275 31.094 59.467 1.00 23.08 5.931 31.265 57.999 1.00 26.36 6.858 32.238 57.324 1.00 26.00 8.075 32.122 57.439 1.00 26.10 6.293 33.210 56.609 1.00 28.94 5.917 29.850 61.588 1.00 22.78 6.445 28.765 61.857 1.00 20.87 .821 30.849 62.461 1.00 23.32 6.322 30.719 63.825 1.00 22.80 6.125 32.046 64.591 1.00 24.62 6.449 31.868 66.076 1.00 24.08 6.997 33.125 63.943 1.00 27.52 6.728 34.543 64.464 1.00 27.69 6.638 29.560 64.573 1.00 22.81 5.294 28.758 65.215 1.00 23.50 4.318 29.463 64.498 1.00 20.16 3.653 28.382 65.186 1.00 18.30 2.125 28.553 65.113 1.00 19.64 1.589 29.739 65.931 1.00 22.60 0.093 29.931 65.623 1.00 24.59 1.759 29.496 67.399 1.00 25.05 4.045 27.028 64.653 1.00 17.14 4.160 26.084 65.436 1.00 18.84 4.225 26.905 63.335 1.00 17.52 4.586 25.591 62.773 1.00 19.05 4.550 25.618 61.241 1.00 19.60 3.167 25.782 60.595 1.00 21.40 3.324 25.870 59.073 1.00 23.62 2.266 24.621 60.975 1.00 21.20 5.968 25.143 63.255 1.00 19.84 6.164 23.977 63.620 1.00 19.38 6.923 26.067 63.269 1.00 20.43 8.270 25.740 63.731 1.00 19.64 9.274 26.881 63.361 1.00 20.44 10.619 26.706 64.102 1.00 20.04 9.486 26.873 61.839 1.00 20.45 10.278 28.076 61.323 1.00 22.03 8.255 25.496 65.239 1.00 19.41 8.894 24.574 65.717 1.00 19.21 7.533 26.322 65.992 1.00 17.59 7.480 26.148 67.446 1.00 19.01 6.624 27.246 68.103 1.00 19.89 6.596 27.154 69.613 1.00 23.82 5.948 28.388 70.243 1.00 26.99 5.645 28.183 71.731 1.00 30.98 ATOM 628 CE LYS 283 6.837 27.917 72.599 1.00 34.38





	ATO		6.873 24.791 67.778 1.00 19.44
	ATOM		7.274 24.120 68.729 1.00 19.31
	ATOM ATOM		5.882 24.390 66.983 1.00 19.18
5	ATOM		5.240 23.124 67.254 1.00 18.56 5.981 21.885 66.806 1.00 18.31
_	ATOM		5.731 20.805 67.328 1.00 19.56
	ATOM	636 N SER 285	6.941 22.024 65.895 1.00 18.65
	ATOM	637 CA SER 285	7.633 20.844 65.384 1.00 17.51
10	ATOM	638 CB SER 285	7.453 20.755 63.870 1.00 19.70
10	ATOM	639 OG SER 285	8.063 21.874 63.212 1.00 18.48
	ATOM ATOM	640 C SER 285	9.136 20.728 65.663 1.00 15.25
	ATOM	641 O SER 285 642 N TRP 286	9.705 19.673 65.406 1.00 15.43 9.770 21.759 66.203 1.00 15.99
	ATOM	643 CA TRP 286	11.221 21.642 66.395 1.00 16.28
15	ATOM	644 CB TRP 286	11.812 22.920 67.007 1.00 17.10
	ATOM	645 CG TRP 286	11.458 23.226 68.414 1.00 17.32
	MOTA	646 CD2 TRP 286	12.117 22.736 69.592 1.00 18.06
	ATOM	647 CE2 TRP 286	11.440 23.291 70.709 1.00 20.12
20	ATOM	648 CE3 TRP 286	13.208 21.882 69.815 1.00 17.92
20	ATOM	649 CD1 TRP 286	10.445 24.033 68.850 1.00 18.61
	MOTA MOTA	650 NE1 TRP 286 651 CZ2 TRP 286	10.427 24.076 70.227 1.00 18.32
	MOTA	652 CZ3 TRP 286	11.816 23.020 72.027 1.00 17.23 13.580 21.608 71.136 1.00 18.42
	ATOM	653 CH2 TRP 286	12.889 22.172 72.219 1.00 19.75
25	ATOM		11.668 20.443 67.219 1.00 16.59
	ATOM	655 O TRP 286	12.655 19.766 66.886 1.00 17.31
	ATOM		10.938 20.167 68.282 1.00 15.26
	ATOM		11.301 19.059 69.157 1.00 14.41
30	ATOM ATOM	658 CB ASN 287 659 CG ASN 287	10.508 19.180 70.456 1.00 17.68
50	ATOM	660 OD1 ASN 287	10.894 18.145 71.474 1.00 19.61 11.757 18.374 72.348 1.00 23.92
	ATOM	661 ND2 ASN 287	10.251 16.991 71.384 1.00 18.83
	ATOM		1.096 17.718 68.448 1.00 14.74
	ATOM	663 O ASN 287 1	11.954 16.846 68.508 1.00 16.16
35	ATOM	664 N GLU 288	9.966 17.555 67.752 1.00 15.22
	ATOM ATOM	665 CA GLU 288	9.745 16.319 66.986 1.00 16.77
	ATOM	666 CB GLU 288 667 CG GLU 288	8.367 16.358 66.288 1.00 17.55 7.213 16.044 67.224 1.00 18.68
	ATOM	668 CD GLU 288	5.868 16.134 66.548 1.00 23.02
40	ATOM	669 OE1 GLU 288	5.786 15.849 65.342 1.00 28.18
	ATOM	670 OE2 GLU 288	4.887 16.461 67.243 1.00 29.07
	ATOM		0.838 16.122 65.921 1.00 17.49
	ATOM		1.338 15.014 65.743 1.00 16.93
45	MOTA		1.193 17.204 65.220 1.00 14.56
43	ATOM ATOM		12.196 17.130 64.173 1.00 15.76 12.248 18.451 63.390 1.00 14.77
	ATOM		11.006 18.639 62.483 1.00 16.67
	ATOM	677 CD1 LEU 289	10.932 20.093 62.002 1.00 18.25
	MOTA		11.083 17.667 61.287 1.00 15.71
50	ATOM	679 C LEU 289 1:	3.555 16.784 64.752 1.00 16.05
	ATOM		4.301 16.022 64.138 1.00 16.56
	ATOM		3.884 17.312 65.929 1.00 16.37
	ATOM ATOM		15.190 16.951 66.529 1.00 16.68 15.477 17.734 67.809 1.00 17.02
55	ATOM		15.786 19.219 67.684 1.00 22.29
-	ATOM		16.294 19.726 69.046 1.00 23.74
	MOTA	686 CD2 LEU 290	16.865 19.454 66.604 1.00 25.08
	ATOM		5.229 15.471 66.868 1.00 16.18



	ATOM	688 O LEU 290	16.214 14.803 66.605 1.00 17.45
	ATOM	689 N LEU 291	14.142 14.958 67.465 1.00 16.16
	ATOM	690 CA LEU 291	14.088 13.553 67.826 1.00 17.64
	MOTA	691 CB LEU 291	12.828 13.289 68.666 1.00 17.32
5	ATOM	692 CG LEU 291	12.824 13.961 70.046 1.00 20.40
	MOTA	693 CD1 LEU 291	11.405 13.964 70.627 1.00 22.18
	ATOM	694 CD2 LEU 291	13.789 13.222 70.971 1.00 23.46
	ATOM	695 C LEU 291	14.087 12.662 66.595 1.00 15.65
	ATOM	696 O LEU 291	14.645 11.569 66.611 1.00 17.39
10	ATOM	697 N PHE 292	13.434 13.116 65.520 1.00 14.81
	ATOM	698 CA PHE 292	13.360 12.330 64.311 1.00 15.62
	ATOM	699 CB PHE 292	12.392 12.993 63.314 1.00 16.43
	ATOM	700 CG PHE 292	12.003 12.113 62.167 1.00 16.59
	ATOM	701 CD1 PHE 292	11.588 10.812 62.389 1.00 18.96
15	ATOM	702 CD2 PHE 292	12.002 12.607 60.875 1.00 19.01
	ATOM	703 CE1 PHE 292	11.170 10.011 61.332 1.00 20.62
	ATOM	704 CE2 PHE 292	11.581 11.805 59.805 1.00 18.46
	MOTA	705 CZ PHE 292	11.166 10.499 60.060 1.00 18.06
	ATOM	706 C PHE 292	14.761 12.191 63.713 1.00 15.70
20	ATOM	707 O PHE 292	15.132 11.119 63.236 1.00 15.72
	ATOM	708 N ALA 293	15.526 13.278 63.760 1.00 16.34
	ATOM	709 CA ALA 293	16.906 13.267 63.232 1.00 16.73
	ATOM	710 CB ALA 293	17.464 14.702 63.207 1.00 17.74
25	ATOM	711 C ALA 293	17.802 12.368 64.090 1.00 17.09 18.668 11.654 63.570 1.00 17.27
25	MOTA	712 O ALA 293 713 N ILE 294	17.623 12.423 65.407 1.00 16.09
	MOTA		18.389 11.569 66.312 1.00 16.22
	MOTA	714 CA ILE 294 715 CB ILE 294	18.032 11.857 67.768 1.00 15.67
	ATOM ATOM	716 CG2 ILE 294	18.584 10.765 68.679 1.00 16.66
30	ATOM	717 CG1 ILE 294	18.615 13.218 68.160 1.00 17.00
30	ATOM	717 COTILE 294	18.206 13.635 69.535 1.00 20.77
	ATOM	719 C ILE 294	18.070 10.111 65.971 1.00 16.74
	ATOM	720 O ILE 294	18.954 9.296 65.833 1.00 16.38
	ATOM	721 N ALA 295	16.791 9.791 65.774 1.00 16.15
35	ATOM	722 CA ALA 295	16.452 8.420 65.424 1.00 16.99
50	ATOM	723 CB ALA 295	14.937 8.273 65.332 1.00 16.54
	ATOM	724 C ALA 295	17.083 7.993 64.088 1.00 17.97
	ATOM	725 O ALA 295	17.563 6.870 63.954 1.00 18.01
	ATOM	726 N TRP 296	17.071 8.881 63.102 1.00 18.59
40	ATOM	727 CA TRP 296	17.625 8.570 61.782 1.00 18.81
	ATOM	728 CB TRP 296	17.321 9.740 60.835 1.00 20.21
	ATOM	729 CG TRP 296	17.849 9.622 59.451 1.00 22.61
	ATOM	730 CD2 TRP 296	17.398 8.716 58.433 1.00 25.62
	MOTA	731 CE2 TRP 296	18.125 9.007 57.265 1.00 26.25
45	MOTA	732 CE3 TRP 296	16.448 7.683 58.402 1.00 25.95
	MOTA	733 CD1 TRP 296	18.807 10.403 58.871 1.00 26.23
	MOTA	734 NE1 TRP 296	18.975 10.043 57.556 1.00 26.50
	MOTA	735 CZ2 TRP 296	17.934 8.297 56.063 1.00 27.77
	ATOM	736 CZ3 TRP 296	16.257 6.977 57.206 1.00 27.65
50	ATOM	737 CH2 TRP 296	16.996 7.289 56.061 1.00 25.35
	ATOM	738 C TRP 296	19.133 8.299 61.878 1.00 19.53
	ATOM	739 O TRP 296	19.647 7.296 61.345 1.00 21.43
	ATOM	740 N ARG 297	19.833 9.147 62.623 1.00 18.58
66	ATOM	741 CA ARG 297	21.280 8.974 62.748 1.00 18.22
55	MOTA	742 CB ARG 297	21.923 10.208 63.376 1.00 18.92 21.886 11.465 62.525 1.00 20.63
	ATOM	743 CG ARG 297	22.792 12.530 63.137 1.00 26.15
	MOTA	744 CD ARG 297 745 NE ARG 297	22.219 13.002 64.381 1.00 29.32
	ATOM	745 NE ARG 297	22.219 13.002 04.301 1.00 29.32

21.393 14.040 64.462 1.00 28.97 ATOM 746 CZ ARG 297 21.066 14.720 63.373 1.00 29.81 747 NH1 ARG 297 20.872 14.372 65.628 1.00 31.03 MOTA 748 NH2 ARG 297 **ATOM** 21.643 7.776 63.605 1.00 18.87 749 C ARG 297 **ATOM** 22.738 7.225 63.473 1.00 19.01 750 O ARG 297 5 **ATOM** 20.749 7.404 64.511 1.00 17.52 751 N SER 298 MOTA 21.023 6.293 65.414 1.00 18.09 752 CA SER 298 **ATOM** 20.134 6.407 66.655 1.00 18.94 753 CB SER 298 20.412 7.606 67.381 1.00 18.16 **MOTA** 754 OG SER 298 ATOM 20.865 4.929 64.770 1.00 20.63 755 C SER 298 MOTA 21.310 3.925 65.336 1.00 24.22 10 756 O SER 298 MOTA 20.270 4.868 63.582 1.00 20.01 757 N MET 299 20.106 3.558 62.953 1.00 22.16 MOTA 758 CA MET 299 19.367 3.682 61.610 1.00 24.42 MOTA 759 CB MET 299 17.940 4.159 61.735 1.00 24.29 MOTA 760 CG MET 299 **MOTA** 17.091 4.052 60.130 1.00 31.30 15 761 SD MET 299 **MOTA** 762 CE MET 299
763 C MET 299
764 O MET 299
765 N GLU 300 18.221 4.950 59.082 1.00 31.06 ATOM 21.431 2.825 62.725 1.00 25.30 21.493 1.600 62.859 1.00 26.84 MOTA **MOTA** 22.485 3.565 62.414 1.00 28.43 23.775 2.944 62.117 1.00 32.11 MOTA 20 766 CA GLU 300 MOTA 24.736 3.949 61.472 1.00 34.60 767 CB GLU 300 MOTA 25.355 4.941 62.420 1.00 40.06 768 CG GLU 300 MOTA 26.689 5.477 61.910 1.00 43.56 769 CD GLU 300 MOTA 27.622 4.666 61.729 1.00 46.83 770 OE1 GLU 300 26.812 6.703 61.688 1.00 45.34 MOTA 25 771 OE2 GLU 300 24.467 2.304 63.300 1.00 32.94 25.389 1.517 63.123 1.00 32.67 24.033 2.649 64.507 1.00 31.51 MOTA 772 C GLU 300 **ATOM** 773 O GLU 300 **ATOM** 774 N PHE 301 **MOTA** 24.632 2.094 65.710 1.00 32.60 775 CA PHE 301 24.822 3.214 66.736 1.00 32.49 30 ATOM 776 CB PHE 301 25.879 4.203 66.349 1.00 34.07 MOTA 777 CG PHE 301 **ATOM** 27.223 3.838 66.358 1.00 33.32 778 CD1 PHE 301 25.537 5.483 65.929 1.00 33.10 **ATOM** 779 CD2 PHE 301 28.207 4.737 65.949 1.00 34.17 **ATOM** 780 CE1 PHE 301 26.506 6.385 65.519 1.00 34.69 **ATOM** 35 781 CE2 PHE 301 **MOTA** 27.854 6.008 65.530 1.00 33.21 781 CE2 PHE 301
782 CZ PHE 301
783 C PHE 301
784 O PHE 301
785 N LEU 302
786 CA LEU 302 MOTA 23.820 0.940 66.301 1.00 33.77 **ATOM** 24.127 0.441 67.377 1.00 34.55 **MOTA** 22.780 0.516 65.589 1.00 34.80 21.966 -0.593 66.045 1.00 36.81 **MOTA** 40 20.641 -0.645 65.287 1.00 34.98 MOTA 787 CB LEU 302 788 CG LEU 302 **ATOM** 19.779 0.596 65.488 1.00 31.61 **ATOM** 18.551 0.528 64.577 1.00 31.62 789 CD1 LEU 302 19.386 0.717 66.955 1.00 31.48 MOTA 790 CD2 LEU 302 22.744 -1.869 65.775 1.00 40.52 MOTA 45 791 C LEU 302 MOTA 23.333 -2.038 64.701 1.00 40.16 792 O LEU 302 22.733 -2.764 66.753 1.00 44.10 MOTA 793 N THR 303 23.422 -4.037 66.634 1.00 48.80 MOTA 794 CA THR 303 **ATOM** 23.126 -4.933 67.850 1.00 49.83 795 CB THR 303 **MOTA** 23.211 -4.151 69.050 1.00 51.18 50 796 OG1 THR 303 MOTA 24.132 -6.076 67.924 1.00 51.25 797 CG2 THR 303 MOTA 22.932 -4.731 65.368 1.00 50.84 798 C THR 303 MOTA 21.739 -4.703 65.052 1.00 50.20 799 O THR 303 23.864 -5.341 64.644 1.00 53.24 MOTA 800 N ALA 304 MOTA 23.538 -6.040 63.410 1.00 55.88 55 801 CA ALA 304 24.739 -6.867 62.946 1.00 56.05 MOTA 802 CB ALA 304 22.317 -6.942 63.575 1.00 57.61 MOTA ATOM 803 C ALA 304





	ATOM 804 O ALA 304 22.133 -7.583 64.617 1.00 58.45	
	21 /81 -6 972 62.540 1.00 59.51	
	ATOM 806 CA ALA 305 20.282 -7.797 62.535 1.00 60.00	
	ATOM 807 CB ALA 305 19.548 -7.657 07.244 1.00 61.71	
5	ATOM 000 0 ALA 205 10 029 63.319 1.00 62.15	
	ATOM 505 31 848 -9 572 62 316 1.00 61.88	
	ATOM 010 010 110 110 110 110 110 110 110 11	
	ATOM 812 C ALA 316 15.833 -9.781 71.403 1.00 57.95	
10	ATOM 813 O ALA 316 15.469 -9.327 70.316 1.00 58.18	
10	ATOM 814 N ALA 316 15.341-12.224 71.575 1.00 58.61	
	ATOM 010 01. 14 247 15 747 -9 096 72.539 1.00 56.79	
	7 739 72 58/ 1.00 54.70	
1.5	ATOM 07 07 ALA 247 13 813 -7 745 73.174 1.00 54.73	
15	ATOM 819 C ALA 317 16.142 -6.871 73.437 1.00 52.91	
	ATOM 820 O ALA 317 15.697 -5.935 74.111 1.00 00.00	
	ATOM 821 N SER 318 17.430 -7.207 73.404 1.00 46.14	
	ATOM 022 07 055 249 49 830 -7 056 73.835 1.00 46.72	
20	ATOM 323 30 SEP 318 20 834 -6 462 74.639 1.00 47.96	
	ATOM 024 00 000 18 378 5 009 73 723 1.00 43.02	
	orb 040 18 6/3 -4 bbb /2.041 1.00 - 1	
	ATOM 827 N PRO 319 18.122 -4.100 74.676 0.56 41.33	
25	ATOM 020 00 DDC 040 18 033 -2 672 74.351 0.50 38.31 ACT	
	ATOM 023 00 000 340 47 690 -2 032 75.694 0.50 38.96 ACT	
	ATOM 030 33 BBQ 340 46 927 -3 116 76.402 0.50 39.34 ACT	
	ATOM 832 C PRO 319 19.310 -2.080 73.730 0.50 35.73 AC1	
30	ATOM 833 O PRO 319 20.394 -2.240 74.519 0.00 30.10	
	ATOM 037 RDQ 320 18 041 -1 404 71.692 1.00 32.09	
	ATOM 000 00 000 20 20 362 -0 784 71,952 1.00 30.83	
	ATOM 000 000 000 10 769 -0 083 70.722 1.00 30.11	
- 35	ATOM 838 CG PRO 320 18.279 -0.174 70.892 1.00 32.74	
- 33	ATOM 839 C PRO 320 21.008 0.185 72.545 1.00 27.36	
	ATOM 840 O PRO 320 20.317 0.624 75.760 1.00 25.76	
	ATOM 041 0301 231 23 060 1.121 73.847 1.00 25.85	
40	ATOM 642 0A 0LN 224 24 262 0 329 74 357 1.00 29.20	
40	ATOM 010 32 024 23 025 -1 090 74./5/ 1.00 34.12	
	ATOM 845 CD GLN 321 23.408 -1.197 76.103 1.00 40.85	
	22 150 -1 617 76.302 1.00 40.57	
	ATOM 071 324 23 546 2 495 73.423 1.00 23.90	
45	ATOM 040 5 CIN 224 23 014 3 297 74.275 1.00 24.10	
	ATOM 070 1 1511 222 23 536 2 790 72.128 1.00 22.59	
	ATOM 851 CA LEU 322 24.050 4.060 71.000 1.00 21.10	
	ATOM 852 CB LEU 322 25.291 3.879 70.770 1100 25.45	
50	A TOW 500 50 1511 202 27 625 3 130 70 345 1.00 28.00	
	ATOM 654 CD0 LEU 322 27 036 4 384 72.497 1.00 24.21	
	ATOM 856 C. LEU 322 23.079 4.942 70.891 1.00 22.08	
	ATOM 857 O LEU 322 22.435 4.478 69.961 1.00 23.11	
5	5 ATOM 858 N MET 323 23.003 6.205 71.270 1.00 23.01	
_	ATOM 859 CA MET 323 22.143 7.157 7.598 1.00 23.20	
	ATOM 800 CD WET 202 20 225 8 922 70 978 1.00 22.36	
	ATOM 861 CG MET 323 20.325 8.922 70.010	

ATOM





19.196 9.636 72.187 1.00 22.04 ATOM 862 SD MET 323 MOTA 863 CE MET 323 18.026 8.314 72.302 1.00 22.12 864 C MET 323 MOTA 23.054 8.187 69.914 1.00 25.54 MOTA 865 O MET 323 24.002 8.691 70.530 1.00 25.31 5 22.781 8.506 68.650 1.00 22.41 MOTA 866 N CYS 324 867 CA CYS 324 23.619 9.483 67.941 1.00 24.83 MOTA 868 CB CYS 324 23.854 9.029 66.512 1.00 23.91 MOTA 869 SG CYS 324 24.921 10.185 65.588 1.00 27.74 MOTA 22.995 10.873 67.950 1.00 24.34 MOTA 870 C CYS 324 22,010 11.148 67.249 1.00 24.90 10 CYS 324 MOTA 871 O 23.560 11.758 68.749 1.00 24.49 872 N LEU 325 ATOM 873 CA LEU 325 23.038 13.114 68.843 1.00 25.66 MOTA 874 CB LEU 325 23.421 13.746 70.183 1.00 26.79 ATOM 875 CG LEU 325 876 CD1 LEU 325 22.935 12.964 71.421 1.00 27.19 MOTA 15 MOTA 23.256 13.744 72.704 1.00 29.28 21.423 12.732 71.320 1.00 27.92 MOTA 877 CD2 LEU 325 878 C LEU 325 23.513 13.990 67.682 1.00 28.10 MOTA 879 O LEU 325 22.860 14.978 67.344 1.00 31.20 MOTA 24.650 13.618 67.094 1.00 28.83 MOTA 880 N MET 326 881 CA MET 326 25.253 14.311 65.947 1.00 30.95 20 MOTA 882 CB MET 326 25.726 15.721 66.350 1.00 31.86 MOTA 26.894 15.710 67.335 1.00 31.84 883 CG MET 326 MOTA MOTA 884 SD MET 326 27.648 17.333 67.693 1.00 34.98 885 CE MET 326 29.085 16.800 68.706 1.00 30.77 MOTA 25 886 C MET 326 26.462 13.453 65.513 1.00 33.06 ATOM 887 O MET 326 MOTA 26.882 12.565 66.242 1.00 32.71 MOTA 888 N PRO 327 27.013 13.682 64.307 1.00 35.54 MOTA 889 CD PRO 327 26.511 14.545 63.227 1.00 35.87 890 CA PRO 327 28.180 12.896 63.857 1.00 36.24 MOTA 891 CB PRO 327 28.508 13.519 62.503 1.00 37.87 30 ATOM 27.159 13.932 62.001 1.00 35.11 892 CG PRO 327 MOTA MOTA 893 C PRO 327 29.353 13.035 64.836 1.00 38.75 894 O PRO 327 29.754 14.154 65.155 1.00 38.99 MOTA 895 N GLY 328 29.890 11.908 65.314 1.00 38.52 MOTA 896 CA GLY 328 31.001 11.933 66.257 1.00 38.65 35 MOTA 897 C GLY 328 30.606 12.217 67.700 1.00 38.39 MOTA GLY 31.431 12.604 68.545 1.00 39.05 898 O 328 MOTA 899 N MET 329 29.326 12.020 67.994 1.00 36.32 MOTA 28.830 12.251 69.326 1.00 34.24 MOTA 900 CA MET 329 28.343 13.693 69.451 1.00 38.91 329 40 MOTA 901 CB MET 27.462 13.991 70.649 1.00 44.24 **MOTA** 902 CG MET 329 MOTA 903 SD MET 329 28.233 13.696 72.235 1.00 50.95 904 CE MET 329 26.854 12.835 73.089 1.00 48.58 MOTA 905 C MET 329 27.700 11.271 69.603 1.00 30.52 **MOTA** 45 **MOTA** 906 O MET 329 26.647 11.331 68.975 1.00 28.92 **MOTA** 907 N THR 330 27.960 10.324 70.490 1.00 26.42 908 CA THR 330 26.933 9.370 70.865 1.00 23.65 **MOTA** 909 CB THR 330 27.338 7.895 70.542 1.00 24.12 MOTA 910 OG1 THR 330 28.672 7.654 71.005 1.00 27.18 MOTA 27.269 7.622 69.034 1.00 26.34 50 911 CG2 THR 330 **ATOM** 26.685 9.475 72.360 1.00 23.23 **ATOM** 912 C THR 330 27,572 9.802 73,146 1.00 23.91 913 O THR 330 MOTA 914 N LEU 331 25.450 9.211 72.748 1.00 20.37 **ATOM** MOTA 915 CA LEU 331 25.082 9.213 74.142 1.00 21.33 23.773 9.986 74.340 1.00 24.38 55 MOTA 916 CB LEU 331 917 CG LEU 331 23.113 9.731 75.696 1.00 25.70 **ATOM** 918 CD1 LEU 331 23.979 10.317 76.825 1.00 30.48 **ATOM** 919 CD2 LEU 331 21.723 10.348 75.694 1.00 29.64





	ATOM 920 C LEU 331 24.892 7.737 74.489 1.00 21.13 ATOM 921 O LEU 331 24.158 7.026 73.819 1.00 19.21 ATOM 922 N HIS 332 25.582 7.262 75.525 1.00 18.80 ATOM 923 CA HIS 332 25.472 5.864 75.901 1.00 18.64 ATOM 924 CB HIS 332 26.740 5.417 76.658 1.00 18.77
5	ATOM 924 CB HIS 332 26.740 5.417 76.656 1.00 21.68 ATOM 925 CG HIS 332 26.826 3.938 76.862 1.00 21.68 ATOM 926 CD2 HIS 332 27.533 2.991 76.205 1.00 22.97 ATOM 927 ND1 HIS 332 26.092 3.273 77.824 1.00 22.38
10	ATOM 928 CE1 HIS 332 26.340 1.978 77.745 1.00 23.74 ATOM 929 NE2 HIS 332 27.213 1.778 76.769 1.00 25.26 ATOM 930 C HIS 332 24.262 5.721 76.820 1.00 18.95 ATOM 931 O HIS 332 23.981 6.620 77.616 1.00 19.91
15	ATOM 933 CA ARG 333 22.394 4.282 77.509 1.00 19.71 ATOM 934 CB ARG 333 21.930 2.850 77.235 1.00 20.65 ATOM 935 CG ARG 333 20.582 2.512 77.896 1.00 21.54 ATOM 936 CD ARG 333 20.018 1.212 77.353 1.00 21.69
20	ATOM 938 CZ ARG 333 18.501 0.034 78.921 1.00 22.46 ATOM 939 NH1 ARG 333 19.535 -0.547 79.531 1.00 24.12 ATOM 940 NH2 ARG 333 17.255 -0.241 79.309 1.00 20.87 ATOM 941 C ARG 333 22.643 4.463 79.018 1.00 21.14
25	ATOM 942 O ARG 333 21.782 4.926 79.733 1.00 21.27 ATOM 943 N ASN 334 23.832 4.107 79.484 1.00 21.27 ATOM 944 CA ASN 334 24.114 4.259 80.910 1.00 23.47 ATOM 945 CB ASN 334 25.486 3.653 81.244 1.00 24.93 ATOM 945 CB ASN 334 25.486 3.653 81.244 1.00 24.93
30	ATOM 947 OD1 ASN 334 24.467 1.461 81.094 1.00 29.08 ATOM 948 ND2 ASN 334 26.707 1.544 81.204 1.00 29.08 ATOM 949 C ASN 334 24.048 5.718 81.380 1.00 22.91 ATOM 950 O ASN 334 23.649 6.000 82.530 1.00 22.99 ATOM 951 N SER 335 24.441 6.657 80.524 1.00 22.89
35	ATOM 952 GA SER 335 25.178 8.915 79.930 1.00 27.35 ATOM 954 OG SER 335 26.517 8.437 79.856 1.00 31.39 ATOM 955 C SER 335 22.908 8.484 80.939 1.00 23.03 ATOM 956 O SER 335 22.496 9.260 81.809 1.00 22.21
40	ATOM 957 N ALA 336 22.126 7.970 79.963 1.00 21.09 ATOM 958 CA ALA 336 20.703 8.255 79.952 1.00 21.09 ATOM 959 CB ALA 336 20.060 7.595 78.718 1.00 21.81 ATOM 960 C ALA 336 20.044 7.744 81.232 1.00 21.37 ATOM 961 O ALA 336 19.209 8.425 81.830 1.00 19.40
45	ATOM 962 N LEU 337 20.423 6.540 81.660 1.00 19.77 19.860 5.960 82.865 1.00 19.59 20.374 4.517 83.039 1.00 19.20 20.374 4.517 83.039 1.00 19.20 20.374 4.517 83.039 1.00 20.97 20.702 2.280 82.055 1.00 23.49 20.702 2.280 82.055 2.002 20.702 2.280 82.055 2.002 20.702 2.280 82.055 2.002 20.002 2
50	ATOM 968 C LEU 337 20.206 6.777 84.089 1.00 20.54 ATOM 969 O LEU 337 19.364 6.997 84.985 1.00 19.57 ATOM 970 N GLN 338 21.454 7.226 84.131 1.00 21.36 ATOM 971 CA GLN 338 21.920 7.994 85.264 1.00 22.39
55	ATOM 972 CB GLN 338 23.439 8.206 85.179 1.00 22.44 ATOM 973 CG GLN 338 23.973 8.755 86.488 1.00 27.14 ATOM 973 CG GLN 338 23.973 8.755 86.481 1.00 29.23





	ATOM 978 O GLN 338 20.894 9.790 86.490 1.00 21.75
	ATOM 980 CA ALA 339 20.215 11.217 84.191 1.00 24.41
5	ATOW 301 301 40 727 11 082 84 463 1.00 24.73
J	ATOM 983 O ALA 339 18.059 12.084 84.041 1.00 22.58
	ATOM 985 CA GLY 340 16.803 9.622 84.754 1.00 23.69
10	ATOM 966 0 021 046 14 666 9 607 83 666 1.00 25.54
10	ATOM 988 N VAL 341 16.492 9.479 82.346 1.00 20.92
	ATOM 990 CB VAL 341 16.134 10.677 80.211 1.00 21.83
1.5	ATOM 992 CG2 VAL 341 17.621 10.577 79.858 1.00 21.51
15	ATOM 993 C VAL 341 15.891 8.183 60.300 1.00 19.53
	ATOM 995 N GLY 342 16.132 7.079 80.999 1.00 19.65
20	ATOM 996 CA GLY 342 16.324 5.527 79.541 1.00 19.27
20	ATOM 998 O GLY 342 15.230 4.771 78.470 1.00 18.82 13.922 5.598 80.088 0.50 18.31 AC1
	ATOM 1000 CA GLN 343 12.706 5.163 79.422 0.50 19.11 ACT
25	ATOM 1001 CB GLN 343 11.307 3.406 79.867 0.50 22.91 AC1
23	ATOM 1003 CD GLN 343 9.082 5.177 80.032 6.00 AC1
	ATOM 1005 NE2 GLN 343 8.606 4.154 81.555 0.50 25.40 AC1
30	ATOM 1000 C GLN 343 12.318 5.127 77.050 0.50 18.83 ACT
30	ATOM 1008 N ILE 344 12.664 7.130 77.37
	ATOM 1000 07 12 344 12.348 9.372 76.875 1.00 18.47 ATOM 1010 CB ILE 344 12.348 9.372 76.875 1.00 20.66
35	ATOM 1012 CG1 ILE 344 11.754 9.984 75.596 1.00 19.04
33	ATOM 1013 CD1 ILE 344 11.445 11.499 75.002 11.00 17.34
	ATOM 1015 O ILE 344 13.440 7.389 74.499 1.00 16.12
40	ATOM 1017 CA PHE 345 15.976 6.826 75.417 1.00 17.85
70	ATOM 1018 CB PHE 345 17.208 6.636 76.522 1.00 18.24
	ATOM 1020 CD1 PHE 345 18.657 4.848 75.273 1.00 18.20
4	ATOM 1021 CB2 FHE 345 19.854 4.412 74.706 1.00 19.01
-T.	ATOM 1023 CE2 PHE 345 20.863 5.673 74.769 1.00 18.58
	ATOM 1025 C PHE 345 15.603 5.522 74.710 1.00 18.98 ATOM 1025 C PHE 345 15.603 5.522 74.710 1.00 18.98
5	ATOM 1026 0 1112 316 15.072 4.568 75.480 1.00 18.04
3	ATOM 1028 CA ASP 346 14.695 3.300 74.697 1.00 19.96
	ATOM 1030 CG ASP 346 15.467 1.768 76.786 1.00 24.04
4	ATOM 1031 OD1 ASP 346 15.232 1.043 77.784 1.00 24.86 55 ATOM 1032 OD2 ASP 346 15.232 1.043 77.784 1.00 18.04
	ATOM 1033 C ASP 346 13.530 3.462 73.841 1.00 19.39
	ATOM 1034 O ASP 346 13.545 2.752 1.00 19.77 ATOM 1035 N ARG 347 12.603 4.359 74.138 1.00 19.77





	ATOM 1036 CA ARG 347 11.493 4.579 73.188 1.00 20.42
	ATOM 1000 047 40 442 5 558 73 708 1.00 24.20
	ATOM 1037 CB ATO 047 0 527 5 024 74 786 1 00 26.30
	ATOM 1030 CD APC 347 8 310 5 929 74.937 1.00 28.76
_	ATOM 1039 NE ARC 347 7 383 5 807 73.813 1.00 29.58
5	6 312 6 577 73.629 1.00 31.91
	ATOM 1042 NH1 ARG 347 6.028 7.536 74.492 1.00 32.14
	ATOM 1043 NH2 ARG 347 5.522 6.378 72.579 1.00 32.47
	ATOM 1044 C ARG 347 12.012 5.120 71.075 1.00 20.00
10	ATOM 1045 C ARC 212 40 020 6 073 71 945 1 00 18 48
	ATOM 1040 IN 17.12 42 420 6 621 70 708 1 00 18.94
	ATOM 1047 OR VAL 348 14 532 7 713 70.991 1.00 18.19
	ATOM 1048 CD41/AL 348 15 286 8 052 69.706 1.00 18.18
15	13.862 8.930 /1.000 1.00 19.11
13	ATOM 1051 C VAL 348 14.143 5.518 69.882 1.00 17.00
	ATOM 1052 O VAL 348 13.885 5.380 68.691 1.00 17.33
	ATOM 1053 N LEU 349 14.981 4.709 70.514 1.00 10.38
	ATOM 1034 CA LEG 049 46 006 3 175 70 526 1 00 20.34
20	ATOM 1033 CO LET 340 17 920 4 286 70.807 1.00 20.49
	ATOM 1057 CD4 LELL 349 19 173 3 626 71.408 1.00 23.32
	ATOM 1057 CD3 LEU 349 18 273 5.078 69.500 1.00 18.92
	ATOM 1059 C LEU 349 14.822 2.509 69.294 1.00 20.39
25	ATOM 1060 O LEU 349 15.112 1.901 66.205 1.00 10.02
	ATOM 1061 N SER 350 13.746 2.206 70.003 1.00.23 27
	ATOM 1002 OR OFF 350 12 443 0 294 70.855 1.00 25.65
	ATOM 1003 OC SER 350 11 622 1 081 71.687 1.00 28.64
20	ATOM 1004 CO SER 350 11.698 1.451 68.766 1.00 21.84
30	ATOM 1066 O SER 350 11.424 0.790 67.762 1.00 25.35
	ATOM 1067 N GLU 351 10.986 2.516 69.131 1.00 22.02
	ATOM 1068 CA GLU 351 3.001 2.002 1.00 22 43
	ATOM 1069 CB GLU 351 8.454 2.916 70.486 1.00 26.86
35	ATOM 1070 CG GLU 351 7.434 3.650 71.303 1.00 28.97
	ATOM 1071 0514 0111 251 7 473 3 544 72.548 1.00 31.85
	ATOM 1073 OF2 GLU 351 6.581 4.330 70.691 1.00 32.66
	ATOM 1074 C GLU 351 10.133 3.708 67.132 1.00 22.11
40	ATOM 1075 O GLU 351 9.348 3.766 07.143 1.00.10 99
	44 606 5 083 65 934 1.00 19.01
	ATOM 1077 OR LEIL 352 12 043 6 555 66.293 1.00 18.64
	ATOM 1076 CO LEU 352 10 911 7.365 66.950 1.00 19.12
45	ATOM 1080 CD1 LEU 352 11.445 8.742 67.339 1.00 19.51
72	ATOM 1081 CD2 LEU 352 9.703 7.505 66.016 1.00 13.20
	ATOM 1082 C LEU 352 12.859 4.467 65.163 1.00 10.01
	ATOM 1003 0 LEG 050 4464 65 754 0 50 18.72
	ATOM 1004 N SER 353 15 203 3 933 65.034 0.50 18.55
5(ATOM 1003 CR CER 353 16.473 4.032 65.883 0.50 16.66
	ATOM 1087 OG SER 353 16.782 5.378 66.160 0.50 11.47
	ATOM 1088 C SER 353 15.045 2.500 64.546 0.50 19.60
	ATOM 1089 O SER 353 15.207 2.236 63.335 0.30 20.25
5	3 ATOM 1090 N 223, 354 44,602 0 181 65 051 1 00 23.55
	ATOM 1091 CR LEU 354 14 360 -0.715 66.278 1.00 24.35
	ATOM 1002 05 1511 054 14 284 2 222 66 012 1.00 30.18
	ATOM 1093 CG LEU 354 14.264 -2.222 35.312 113

AC1 AC1 AC1 AC1 AC1 AC1





	ATOM 1094 CD1 LEU 354 15.388 -2.664 65.055 1.00 31.88
	ATOM 1095 CD2 LEU 354 14.392 -2.944 67.345 1.00 31.36
	ATOM 1095 CD2 EEU 354 13.489 -0.011 64.009 1.00 24.82 ATOM 1096 C LEU 354 13.489 -0.011 64.009 1.00 25.66
	ATOM 1098 C LEG 354 ATOM 1097 O LEU 354 13.696 -0.684 63.004 1.00 25.66 ATOM 1098 N LYS 355 12.324 0.587 64.234 1.00 26.97
5	ATOM 1000 TE 1100 26 95
	ATOM 1099 CA 113 355 40.003 1.226 63.735 1.00.29.30
	ATOM 1100 CB 1100 355 0 328 0 572 64 843 1 00 34 34
	ATOM 1103 CD LVS 355 8 440 -0.616 64.321 1.00 38.57
10	ATOM 1103 CE LVS 355 7 365 -1.007 65.319 1.00 39.54
10	ATOM 4404 NZ LVS 355 7 883 -0.958 66./13 1.00 40.20
	ATOM 1105 C LYS 355 11.637 0.964 61.899 1.00 27.30
	ATOM 1105 C LTG 355 11.281 0.369 60.883 1.00 28.58 ATOM 1107 N MET 356 12.362 2.080 61.860 1.00 25.41
	ATOM 1107 N 155 12 797 2 641 60 594 1 00 25 37
15	ATOM 1100 07 1157 050 40 270 4071 60 778 1 00 27 04
	ATOM TIO9 CB WILT 330 10.26 57
	ATOM 1111 SD MET 356 12 669 6.671 60.768 1.00 36.72
	ATOM 1112 CF MFT 356 13.015 6.835 62.357 1.00 16.80
20	ATOM 1113 C MET 356 13.836 1.808 59.896 1.00 26.93
20	ATOM 1114 O MET 356 13.907 1.807 58.676 1.00 25.41
	ATOM 1115 N ARG 357 14.672 1.114 60.661 1.00 27.66
	ATOM 1110 07. 1557 40 722 0 214 60 961 1 00 31 09
	A OM 1117 CB ARG 557 10:100 0:12
25	ATOM 1118 CG ARG 357 18.840 -1.607 61.112 1.00 38.46
	ATOM 1120 NE ARG 357 18.313 -2.543 62.097 1.00 41.53
	ATOM 1131 C7 ARG 357 19 066 -3.164 63.003 1.00 43.38
	ATOM 4422 NH4 APG 357 20 376 -2.942 63.037 1.00 42.92
30	ATOM 1123 NH2 ARG 357 18.512 -3.995 63.879 1.00 43.40
	ATOM 1124 C ARG 357 14.926 -0.925 59.422 1.00 29.63 ATOM 1125 O ARG 357 15.218 -1.353 58.310 1.00 29.83
	40.000 4.452 60.171 1.00.29.51
	40.004 2.600 50.704 1.00.30.65
35	12 273 -3 117 60.812 1.00 31.00
33	ATOM 4420 OG1 THR 358 13 071 -3.609 61.895 1.00 32.46
	ATOM 1130 CG2 THR 358 11.374 -4.260 60.306 1.00 34.26
	ATOM 1131 C THR 358 12.408 -2.281 58.438 1.00 30.73
	ATOM 1132 O THE 330 14.005 4.050 59.350 1.00.29.40
40	ATOM 1133 N LEG 333 14.404 0.610 57.201 1.00.29.68
	40.040 0.502 57.605 1.00.30.32
	ATOM 1136 CG LEIL 359 8 732 0.609 57.321 1.00 34.26
	ATOM 1137 CD1 LEU 359 8.197 2.038 57.529 1.00 33.77
45	ATOM 4439 CD3 LEIL 359 8 452 0.142 55.900 1.00 34.00
	ATOM 1139 C LEU 359 12.046 -0.168 56.066 1.00 20.77
	ATOM 1140 O LEU 359 11.585 0.164 54.974 1.00 27.30
	710W 1111 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
~ ~	ATOM 1142 077 7110 14 1004 0 505 54 178 1 00 33 80
50	ATOM 1144 CG ARG 360 14.798 -2.076 54.625 1.00 36.43
	ATOM 1145 CD ARG 360 14.018 -3.165 53.900 1.00 39.56
	ATOM 1146 NE ARG 360 12.588 -3.168 54.226 1.00 41.14
	ATOM 1147 CZ ARG 360 11.618 -2.942 53.340 1.00 42.18
55	ATOM 1148 NH1 ARG 360 11.918 -2.688 52.071 1.00 41.02
	42.075 1.600 54.787 1.00.29.92
	ATOM 1100 0 7100 000 44 073 1 058 53 592 1 00 28 84
	ATOM 1151 O ARG 360 14.073 1.958 53.592 1.00 26.04

ATOM 1152 N VAL 361

ATOM 1153 CA VAL 361

ATOM 1154 CB VAL 361

ATOM 1155 CG1 VAL 361

ATOM 1156 CG2 VAL 361

ATOM 1157 C VAL 361

ATOM 1158 O VAL 361

ATOM 1159 N ASP 362

ATOM 1160 CA ASP 362

ATOM 1161 CB ASP 362

ATOM 1162 CG ASP 362

ATOM 1163 OD1 ASP 362

ATOM 1165 C ASP 362

ATOM 1166 O ASP 362

ATOM 1167 N GLN 363

ATOM 1168 CA GLN 363 ATOM 1169 CB GLN 363

ATOM 1170 CG GLN 363

ATOM 1174 C GLN 363

ATOM 1175 O GLN 363 ATOM 1176 N ALA 364

ATOM 1177 CA ALA 364

ATOM 1178 CB ALA 364

ATOM 1179 C ALA 364

ATOM 1180 O ALA 364

ATOM 1181 N GLU 365

ATOM 1204 CB VAL 367

ATOM 1205 CG1 VAL 367

ATOM 1206 CG2 VAL 367

ATOM 1207 C VAL 367

ATOM 1208 O VAL 367

ATOM 1209 N ALA 368

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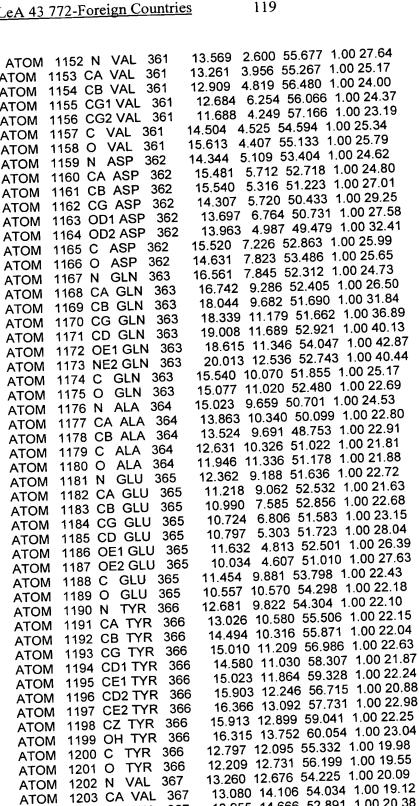
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13.955 14.666 52.891 1.00 20.38

15.446 14.473 53.249 1.00 21.37

13.609 14.009 51.554 1.00 19.90

11.607 14.458 53.784 1.00 18.65

11.165 15.538 54.178 1.00 18.48

10.868 13.552 53.147 1.00 20.47



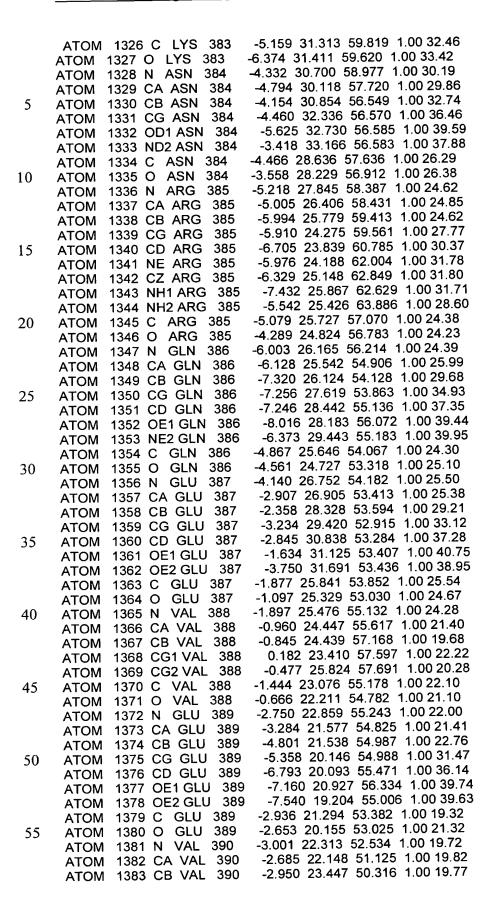


5	ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1211 CB ALA 368 1212 C ALA 368 1213 O ALA 368 1214 N LEU 369 1215 CA LEU 369 1216 CB LEU 369	9.447 13.787 52.893 1.00 19.05 8.854 12.668 51.988 1.00 18.93 8.714 13.813 54.240 1.00 19.17 7.863 14.682 54.487 1.00 18.81 9.048 12.871 55.112 1.00 19.43 8.417 12.819 56.428 1.00 17.85 8.807 11.526 57.147 1.00 20.14
10	ATOM ATOM ATOM ATOM	1217 CG LEU 369 1218 CD1 LEU 369 1219 CD2 LEU 369 1220 C LEU 369 1221 O LEU 369	8.153 10.250 56.565 1.00 21.25 8.810 9.041 57.154 1.00 22.02 6.626 10.219 56.856 1.00 21.64 8.772 14.076 57.235 1.00 19.07 7.945 14.606 57.965 1.00 17.17
15	ATOM ATOM ATOM ATOM ATOM	1222 N LYS 370 1223 CA LYS 370 1224 CB LYS 370 1225 CG LYS 370 1226 CD LYS 370	10.007 14.567 57.120 1.00 18.01 10.363 15.799 57.826 1.00 19.26 11.819 16.199 57.522 1.00 18.97 12.888 15.349 58.203 1.00 21.31 14.304 15.860 57.845 1.00 25.49 14.445 17.367 58.009 1.00 25.79
20	ATOM ATOM ATOM ATOM ATOM	1227 CE LYS 370 1228 NZ LYS 370 1229 C LYS 370 1230 O LYS 370 1231 N ALA 371	15.878 17.841 57.879 1.00 29.87 9.440 16.949 57.388 1.00 17.68 8.950 17.717 58.203 1.00 17.05 9.209 17.075 56.081 1.00 17.98
25	ATOM ATOM ATOM ATOM	1232 CA ALA 371 1233 CB ALA 371 1234 C ALA 371 1235 O ALA 371 1236 N ILE 372	8.368 18.154 55.596 1.00 17.26 8.344 18.154 54.065 1.00 19.00 6.957 17.957 56.140 1.00 15.65 6.299 18.909 56.533 1.00 17.13 6.492 16.713 56.151 1.00 14.92
30	MOTA ATOM ATOM ATOM MOTA	1237 CA ILE 372 1238 CB ILE 372 1239 CG2 ILE 372 1240 CG1 ILE 372 1241 CD1 ILE 372	5.146 16.450 56.673 1.00 16.38 4.743 14.956 56.430 1.00 15.28 3.477 14.602 57.245 1.00 17.98 4.566 14.730 54.915 1.00 18.14 4.413 13.271 54.530 1.00 18.13
35	ATOM ATOM ATOM ATOM ATOM	1242 C ILE 372 1243 O ILE 372 1244 N ILE 373 1245 CA ILE 373 1246 CB ILE 373	5.038 16.795 58.163 1.00 16.98 4.028 17.317 58.606 1.00 16.87 6.089 16.522 58.942 1.00 14.47 6.080 16.829 60.369 1.00 15.13 7.392 16.251 61.042 1.00 13.81
40	ATOM ATOM ATOM ATOM ATOM	1247 CG2 ILE 373 1248 CG1 ILE 373 1249 CD1 ILE 373 1250 C ILE 373 1251 O ILE 373	7.530 16.783 62.463 1.00 15.08 7.340 14.717 61.052 1.00 14.66 8.709 14.031 61.219 1.00 17.60 5.962 18.350 60.604 1.00 15.01 5.212 18.817 61.477 1.00 15.67
45	ATOM ATOM ATOM ATOM ATOM	1252 N LEU 374 1253 CA LEU 374 1254 CB LEU 374 1255 CG LEU 374 1256 CD1 LEU 374	6.702 19.109 59.796 1.00 16.23 6.688 20.557 59.880 1.00 15.91 7.738 21.160 58.942 1.00 18.27 7.702 22.700 58.759 1.00 19.49 8.184 23.403 60.044 1.00 18.70
50	MOTA MOTA MOTA MOTA	1257 CD2 LEU 374 1258 C LEU 374 1259 O LEU 374 1260 N LEU 375 1261 CA LEU 375	8.596 23.092 57.597 1.00 19.61 5.316 21.128 59.490 1.00 17.14 4.765 21.980 60.167 1.00 16.72 4.803 20.662 58.367 1.00 17.78 3.561 21.202 57.831 1.00 17.01
55	ATOM ATOM ATOM ATOM ATOM ATOM	1262 CB LEU 375 1263 CG LEU 375 1264 CD1 LEU 375 1265 CD2 LEU 375 1266 C LEU 375 1267 O LEU 375	3.573 21.071 56.301 1.00 19.06 4.788 21.715 55.581 1.00 18.84 4.903 21.197 54.151 1.00 18.22 4.644 23.234 55.610 1.00 19.41 2.349 20.514 58.422 1.00 19.26 1.603 19.823 57.705 1.00 19.50





ATOM 1268 N ASN 376 2.178 20.727 59.723 1.00 16.95 ATOM 1269 CA ASN 376 1.087 20.136 60.510 1.00 19.78 ATOM 1270 CB ASN 376 1.605 19.772 61.912 1.00 18.97 ATOM 1271 CG ASN 376 0.537 19.124 62.780 1.00 23.13 5 ATOM 1272 OD1 ASN 376 -0.527 18.732 62.289 1.00 19.72 ATOM 1273 ND2 ASN 376 0.827 18.989 64.081 1.00 21.10 ATOM 1274 C ASN 376 -0.088 21.080 60.641 1.00 17.80 ATOM 1275 O ASN 376 -0.043 22.028 61.412 1.00 18.77 ATOM 1276 N PRO 377 -1.188 20.820 59.909 1.00 20.03 ATOM 1277 CD PRO 377 -1.463 19.684 59.010 1.00 19.34 10 -2.342 21.728 60.011 1.00 20.40 ATOM 1278 CA PRO 377 ATOM 1279 CB PRO 377 -3.239 21.293 58.858 1.00 18.78 ATOM 1280 CG PRO 377 -2.979 19.796 58.774 1.00 19.22 ATOM 1281 C PRO 377 -3.086 21.705 61.336 1.00 21.89 ATOM 1282 O PRO 377 15 -3.922 22.583 61.594 1.00 22.57 ATOM 1283 N ASP 378 -2.771 20.723 62.177 1.00 20.09 ATOM 1284 CA ASP 378 -3.444 20.609 63.463 1.00 22.47 ATOM 1285 CB ASP 378 -3.608 19.131 63.809 1.00 23.71 -4.555 18.426 62.847 1.00 25.43 -5.579 19.028 62.487 1.00 28.35 ATOM 1286 CG ASP 378 20 ATOM 1287 OD1 ASP 378 ATOM 1288 OD2 ASP 378 -4.289 17.283 62.443 1.00 30.58 ATOM 1289 C ASP 378 -2.823 21.403 64.603 1.00 22.30 ATOM 1290 O ASP 378 ATOM 1291 N VAL 379 -3.265 21.309 65.760 1.00 22.98 -1.793 22.181 64.279 1.00 22.51 ATOM 1292 CA VAL 379 25 -1.167 23.053 65.266 1.00 21.52 ATOM 1293 CB VAL 379 0.044 23.807 64.662 1.00 20.60 0.424 25.004 65.532 1.00 22.27 ATOM 1294 CG1 VAL 379 1.226 22.848 64.516 1.00 22.31 ATOM 1295 CG2 VAL 379 ATOM 1296 C VAL 379 -2.255 24.048 65.658 1.00 23.83 30 ATOM 1297 O VAL 379 -2.918 24.655 64.793 1.00 25.06 ATOM 1298 N LYS 380 -2.460 24.212 66.958 1.00 23.33 ATOM 1299 CA LYS 380 -3.490 25.124 67.430 1.00 24.49 ATOM 1300 CB LYS 380 -3.797 24.829 68.904 1.00 25.21 ATOM 1301 CG LYS 380 -4.182 23.365 69.131 1.00 28.03 ATOM 1302 CD LYS 380 -4.460 23.035 70.594 1.00 30.82 35 ATOM 1303 CE LYS 380 -4.728 21.536 70.758 1.00 31.68 -4.904 21.079 72.177 1.00 33.50 ATOM 1304 NZ LYS 380 ATOM 1305 C LYS 380 -3.055 26.573 67.250 1.00 24.85 ATOM 1306 O LYS 380 -1.874 26.891 67.408 1.00 25.55 ATOM 1307 N GLY 381 -3.988 27.445 66.861 1.00 24.69 40 ATOM 1308 CA GLY 381 -3.647 28.852 66.704 1.00 26.29 ATOM 1309 C GLY 381 ATOM 1310 O GLY 381 ATOM 1311 N LEU 382 -3.384 29.378 65.295 1.00 25.30 -3.246 30.598 65.093 1.00 27.29 -3.313 28.490 64.311 1.00 26.35 ATOM 1312 CA LEU 382 45 -3.054 28.914 62.941 1.00 26.95 ATOM 1313 CB LEU 382 -2,997 27,706 61,995 1,00 25,01 ATOM 1314 CG LEU 382 -1.865 26.700 62.265 1.00 24.87 ATOM 1315 CD1 LEU 382 -2.011 25.507 61.314 1.00 24.53 ATOM 1316 CD2 LEU 382 -0.518 27.384 62.064 1.00 24.40 ATOM 1317 C LEU 382 -4.120 29.885 62.428 1.00 28.77 50 ATOM 1318 O LEU 382 -5.310 29.719 62.695 1.00 28.39 ATOM 1319 N LYS 383 -3.660 30.881 61.681 1.00 30.83 ATOM 1320 CA LYS 383 -4.518 31.894 61.078 1.00 32.60 -3.670 33.104 60.699 1.00 35.65 ATOM 1321 CB LYS 383 ATOM 1322 CG LYS 383 -4.352 34.121 59.788 1.00 40.31 55 -5.044 35.203 60.589 1.00 42.92 ATOM 1323 CD LYS 383 -5.436 36.376 59.702 1.00 43.80 ATOM 1324 CE LYS 383 ATOM 1325 NZ LYS 383 -6.040 37.476 60.505 1.00 44.52



ATOM 1391 CG LEU 391

ATOM 1392 CD1 LEU 391

ATOM 1393 CD2 LEU 391

ATOM 1396 N ARG 392

ATOM 1397 CA ARG 392

ATOM 1397 CA ARG 392 ATOM 1398 CB ARG 392 ATOM 1399 CG ARG 392 ATOM 1400 CD ARG 392 ATOM 1401 NE ARG 392

ATOM 1406 O ARG 392

ATOM 1407 N GLU 393

ATOM 1408 CA GLU 393

ATOM 1409 CB GLU 393

ATOM 1410 CG GLU 393

ATOM 1411 CD GLU 393

ATOM 1413 OLZ GLU 393 ATOM 1415 O GLU 393 ATOM 1416 N LYS 394

ATOM 1417 CA LYS 394

ATOM 1418 CB LYS 394

ATOM 1422 NZ LYS 394

ATOM 1423 C LYS 394

ATOM 1424 O LYS 394

ATOM 1425 N MET 395

ATOM 1437 CD1 PHE 396

ATOM 1438 CD2 PHE 396

ATOM 1439 CE1 PHE 396

ATOM 1440 CE2 PHE 396

ATOM 1441 CZ PHE 396

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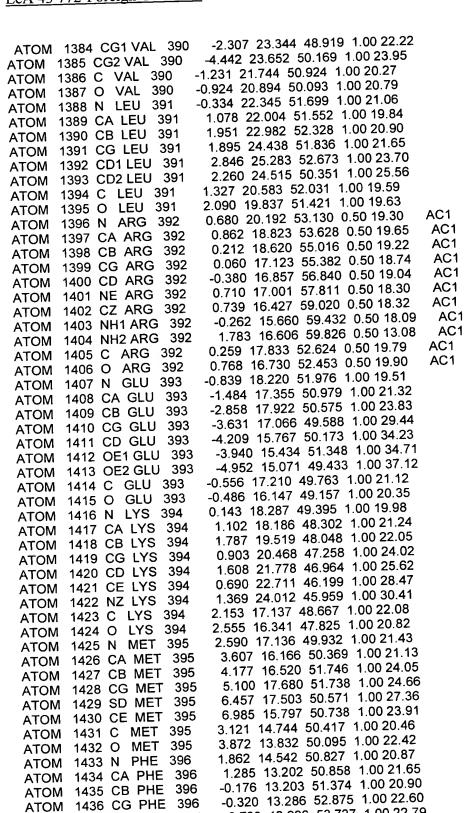
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0.570 13.063 55.116 1.00 20.29

-1.712 13.702 54.826 1.00 23.72

-0.655 13.416 55.669 1.00 22.24

AC1 AC1 AC1 AC1 AC1

ATOM 1442 C PHE 396

ATOM 1443 O PHE 396

ATOM 1444 N LEU 397

ATOM 1445 CA LEU 397

ATOM 1446 CB LEU 397

ATOM 1447 CG LEU 397

ATOM 1448 CD1 LEU 397

ATOM 1449 CD2 LEU 397

ATOM 1450 C LEU 397

ATOM 1451 O LEU 397

ATOM 1452 N CYS 398 ATOM 1453 CA CYS 398

ATOM 1454 CB CYS 398

ATOM 1455 SG CYS 398

ATOM 1456 C CYS 398

ATOM 1457 O CYS 398 ATOM 1458 N LEU 399

ATOM 1459 CA LEU 399

ATOM 1460 CB LEU 399

ATOM 1461 CG LEU 399

ATOM 1462 CD1 LEU 399

ATOM 1463 CD2 LEU 399

ATOM 1464 C LEU 399

ATOM 1465 O LEU 399

ATOM 1466 N ASP 400

ATOM 1467 CA ASP 400

ATOM 1468 CB ASP 400

ATOM 1469 CG ASP 400

ATOM 1470 OD1 ASP 400 ATOM 1471 OD2 ASP 400

ATOM 1473 O ASP 400

ATOM 1474 N GLU 401

ATOM 1475 CA GLU 401

ATOM 1476 CB GLU 401

ATOM 1477 CG GLU 401 ATOM 1478 CD GLU 401

ATOM 1479 OE1 GLU 401

ATOM 1480 OE2 GLU 401

ATOM 1481 C GLU 401

ATOM 1482 O GLU 401 ATOM 1483 N TYR 402

ATOM 1484 CA TYR 402

ATOM 1485 CB TYR 402 ATOM 1486 CG TYR 402

ATOM 1488 CE1 TYR 402 ATOM 1489 CD2 TYR 402

ATOM 1490 CE2 TYR 402 ATOM 1491 CZ TYR 402

ATOM 1492 OH TYR 402

ATOM 1493 C TYR 402

ATOM 1494 O TYR 402

ATOM 1495 N CYS 403

ATOM 1496 CA CYS 403

ATOM 1497 CB CYS 403

ATOM 1498 SG CYS 403

ATOM 1499 C CYS 403

1487 CD1 TYR 402

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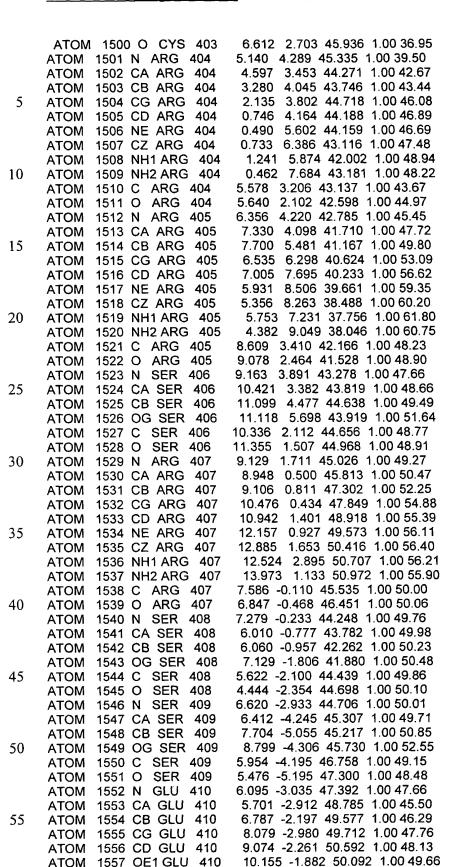
MOTA



1.281 12.652 49.429 1.00 22.43 1.635 11.494 49.215 1.00 21.80 0.844 13.462 48.458 1.00 22.96 0.813 13.022 47.061 1.00 21.97 0.139 14.099 46.176 1.00 22.88 -1.385 14.161 46.354 1.00 23.93 -1.981 15.078 45.315 1.00 25.27 -1.972 12.759 46.190 1.00 25.99 2.233 12.705 46.560 1.00 24.94 2.450 11.692 45.873 1.00 25.61 3.195 13.548 46.924 1.00 23.80 4.593 13.333 46.519 1.00 26.51 5.509 14.454 47.041 1.00 28.87 5.551 15.910 46.032 1.00 39.48 5.111 12.027 47.090 1.00 25.35 5.738 11.221 46.399 1.00 25.03 4.861 11.821 48.371 1.00 24.81 5.366 10.620 49.009 1.00 24.04 5.232 10.739 50.530 1.00 24.26 5,806 9,580 51,344 1,00 24,01 7.281 9.343 50.985 1.00 22.08 5.672 9.931 52.821 1.00 22.85 4.715 9.352 48.518 1.00 26.35 5.398 8.363 48.267 1.00 25.02 3.391 9.377 48.361 1.00 27.30 2.680 8.200 47.874 1.00 29.09 1.179 8.490 47.772 1.00 31.25 0.379 7.258 47.400 1.00 34.75 0.236 6.356 48.252 1.00 35.16 -0.091 7.188 46.250 1.00 38.49 ATOM 1472 C ASP 400 3.217 7.816 46.497 1.00 28.91 3.436 6.642 46.212 1.00 29.66 3.420 8.813 45.644 1.00 28.16 3,936 8.577 44.299 1.00 29.87 4.052 9.895 43.533 1.00 32.50 4.735 9.751 42.180 1.00 38.83 4.784 11.048 41.406 1.00 42.93 5,449 12.003 41.865 1.00 45.46 4,147 11.114 40.334 1.00 45.87 5.308 7.911 44.360 1.00 31.19 5.574 6.926 43.650 1.00 31.37 6.171 8.444 45.224 1.00 28.55 7.516 7.918 45.365 1.00 29.01 8.314 8.737 46.384 1.00 27.40 9.667 8.134 46.659 1.00 27.45 9.849 7.238 47.709 1.00 27.18 11.087 6.635 47.933 1.00 28.15 10.747 8.419 45.834 1.00 27.22 11.996 7.820 46.050 1.00 30.03 12.147 6.936 47.097 1.00 30.78 13.374 6.358 47.316 1.00 31.66 7.503 6.453 45.769 1.00 30.16 8.206 5.641 45.187 1.00 29.67 6.700 6.113 46.763 1.00 30.42 6.616 4.739 47.215 1.00 34.32 5,691 4.650 48.430 1.00 33.37

6.357 5.485 49.920 1.00 31.63

6.116 3.820 46.104 1.00 36.81







ATOM 1558 OE2 GLU 410 8,761 -2.063 51.784 1.00 48.57 ATOM 1559 C GLU 410 4.373 -2.197 48.973 1.00 44.10 ATOM 1560 O GLU 410 4.311 -0.974 49.114 1.00 41.70 ATOM 1561 N GLU 411 3.306 -2.985 48.986 1.00 42.76 1.973 -2.451 49.154 1.00 41.57 5 ATOM 1562 CA GLU 411 ATOM 1563 CB GLU 411 0.945 -3.529 48.814 1.00 44.42 ATOM 1564 CG GLU 411 1.166 -4.132 47.439 1.00 48.49 ATOM 1565 CD GLU 411 0.151 -5.191 47.100 1.00 49.60 0.111 -6.226 47.806 1.00 49.80 ATOM 1566 OE1 GLU 411 -0.605 -4.979 46.129 1.00 50.58 ATOM 1567 OE2 GLU 411 10 1.805 -2.000 50.594 1.00 38.78 ATOM 1568 C GLU 411 2.254 -2.682 51.526 1.00 38.53 ATOM 1569 O GLU 411 1.170 -0.845 50.768 1.00 34.78 ATOM 1570 N GLY 412 0.953 -0.313 52.103 1.00 32.19 ATOM 1571 CA GLY 412 ATOM 1572 C GLY 412 2.163 0.402 52.695 1.00 29.28 15 ATOM 1573 O GLY 412 2.133 0.770 53.865 1.00 28.68 ATOM 1574 N ARG 413 3.207 0.625 51.901 1.00 28.70 4.413 1.286 52.407 1.00 27.65 ATOM 1575 CA ARG 413 5.513 1.319 51.348 1.00 29.50 ATOM 1576 CB ARG 413 6.850 1.839 51.905 1.00 29.56 ATOM 1577 CG ARG 413 20 8.004 1.721 50.903 1.00 32.68 ATOM 1578 CD ARG 413 9.242 2.244 51.484 1.00 34.48 ATOM 1579 NE ARG 413 9.951 1.632 52.433 1.00 35.49 ATOM 1580 CZ ARG 413 ATOM 1581 NH1 ARG 413 9,569 0.454 52.914 1.00 34.87 11.036 2.221 52.929 1.00 35.73 ATOM 1582 NH2 ARG 413 25 ATOM 1583 C ARG 413 4.153 2.715 52.874 1.00 27.61 4.656 3.142 53.911 1.00 26.64 ATOM 1584 O ARG 413 ATOM 1585 N PHE 414 3.377 3.447 52.091 1.00 27.23 3.025 4.829 52.406 1.00 25.72 ATOM 1586 CA PHE 414 2.109 5.368 51.290 1.00 27.69 ATOM 1587 CB PHE 414 30 1.553 6.756 51.552 1.00 26.95 ATOM 1588 CG PHE 414 2.359 7.882 51.454 1.00 28.43 ATOM 1589 CD1 PHE 414 0.217 6.921 51.891 1.00 29.19 ATOM 1590 CD2 PHE 414 1.842 9.165 51.692 1.00 28.49 ATOM 1591 CE1 PHE 414 ATOM 1592 CE2 PHE 414 -0.315 8.199 52.134 1.00 29.46 35 ATOM 1593 CZ PHE 414 0,503 9.325 52.033 1.00 28.75 2.336 4.891 53.777 1.00 26.40 ATOM 1594 C PHE 414 2.691 5.702 54.637 1.00 26.65 ATOM 1595 O PHE 414 1.355 4.027 53.997 1.00 25.07 ATOM 1596 N ALA 415 0.652 4.002 55.271 1.00 24.63 ATOM 1597 CA ALA 415 40 -0.531 3.028 55.193 1.00 23.72 ATOM 1598 CB ALA 415 1.572 3.622 56.436 1.00 24.02 ATOM 1599 C ALA 415 1,433 4,142 57,547 1.00 23,15 ATOM 1600 O ALA 415 2.518 2.722 56.174 1.00 24.35 ATOM 1601 N ALA 416 3.448 2.270 57.205 1.00 24.54 ATOM 1602 CA ALA 416 45 4.313 1.143 56.666 1.00 24.42 ATOM 1603 CB ALA 416 4.319 3.436 57.639 1.00 23.97 ATOM 1604 C ALA 416 4.544 3.646 58.832 1.00 25.89 ATOM 1605 O ALA 416 4.799 4.192 56.664 1.00 23.99 ATOM 1606 N LEU 417 ATOM 1607 CA LEU 417 5,638 5.348 56.952 1.00 23.65 50 6.056 6.013 55.651 1.00 23.88 ATOM 1608 CB LEU 417 6.940 5.132 54.768 1.00 22.81 ATOM 1609 CG LEU 417 7.104 5.745 53.381 1.00 25.97 ATOM 1610 CD1 LEU 417 8.313 4.978 55.464 1.00 24.86 ATOM 1611 CD2 LEU 417 4,894 6.346 57.843 1.00 23.64 ATOM 1612 C LEU 417 55 5.434 6.825 58.851 1.00 24.26 ATOM 1613 O LEU 417 3.635 6.632 57.517 1.00 22.96 ATOM 1614 N LEU 418 2.896 7.617 58.305 1.00 22.78 ATOM 1615 CA LEU 418



127 555 7.961 57.622 1.00 22

1.555 7.961 57.622 1.00 22.19 ATOM 1616 CB LEU 418 1.632 8.536 56.193 1.00 22.93 ATOM 1617 CG LEU 418 0.232 8.983 55.715 1.00 23.88 ATOM 1618 CD1 LEU 418 2.554 9.749 56.179 1.00 23.65 ATOM 1619 CD2 LEU 418 2.646 7.201 59.762 1.00 24.12 ATOM 1620 C LEU 418 2.372 8.046 60.620 1.00 22.61 5 ATOM 1621 O LEU 418 2.706 5.901 60.049 1.00 25.06 ATOM 1622 N LEU 419 2.496 5.440 61.404 1.00 27.92 ATOM 1623 CA LEU 419 2.406 3.909 61.451 1.00 31.65 ATOM 1624 CB LEU 419 1.114 3.343 60.884 1.00 34.11 ATOM 1625 CG LEU 419 1.026 1.848 61.218 1.00 36.06 10 ATOM 1626 CD1 LEU 419 -0.068 4.081 61.480 1.00 34.83 ATOM 1627 CD2 LEU 419 3.594 5.891 62.360 1.00 29.85 ATOM 1628 C LEU 419 3.400 5.885 63.574 1.00 31.55 ATOM 1629 O LEU 419 4.736 6.296 61.828 1.00 31.33 ATOM 1630 N ARG 420 5.801 6.725 62.718 1.00 31.87 15 ATOM 1631 CA ARG 420 7.145 6.755 61.985 1.00 32.74 ATOM 1632 CB ARG 420 7.648 5.387 61.490 1.00 33.67 ATOM 1633 CG ARG 420 7.856 4.364 62.622 1.00 36.93 ATOM 1634 CD ARG 420 6.709 3.481 62.820 1.00 35.35 ATOM 1635 NE ARG 420 6.179 3.194 64.003 1.00 37.82 20 ATOM 1636 CZ ARG 420 6.692 3.714 65.116 1.00 39.26 ATOM 1637 NH1 ARG 420 5.112 2.408 64.079 1.00 39.04 ATOM 1638 NH2 ARG 420 5.477 8.092 63.303 1.00 32.15 ATOM 1639 C ARG 420 5.995 8.456 64.362 1.00 31.60 ATOM 1640 O ARG 420 4.591 8.845 62.655 1.00 30.38 25 ATOM 1641 N LEU 421 4.278 10.175 63.164 1.00 29.53 ATOM 1642 CA LEU 421 3.519 10.976 62.121 1.00 30.72 ATOM 1643 CB LEU 421 4.322 11.027 60.808 1.00 31.31 ATOM 1644 CG LEU 421 3.645 12.019 59.885 1.00 32.38 ATOM 1645 CD1 LEU 421 5.800 11.411 61.053 1.00 31.74 30 ATOM 1646 CD2 LEU 421 3.582 10.256 64.521 1.00 28.39 ATOM 1647 C LEU 421 3.977 11.061 65.363 1.00 26.36 ATOM 1648 O LEU 421 2.533 9.446 64.762 1.00 27.69 ATOM 1649 N PRO 422 1.678 8.672 63.839 1.00 27.47 ATOM 1650 CD PRO 422 1.915 9.559 66.090 1.00 26.04 35 ATOM 1651 CA PRO 422 0.717 8.603 66.005 1.00 28.29 ATOM 1652 CB PRO 422 0.350 8.664 64.557 1.00 28.91 ATOM 1653 CG PRO 422 2.906 9.143 67.198 1.00 25.36 ATOM 1654 C PRO 422 2.832 9.637 68.322 1.00 24.06 ATOM 1655 O PRO 422 3.821 8.228 66.872 1.00 24.34 40 ATOM 1656 N ALA 423 4.817 7.779 67.840 1.00 22.88 ATOM 1657 CA ALA 423 5.589 6.599 67.273 1.00 26.29 ATOM 1658 CB ALA 423 5.765 8.942 68.158 1.00 24.20 ATOM 1659 C ALA 423 6.094 9.197 69.315 1.00 22.14 ATOM 1660 O ALA 423 6.212 9.640 67.119 1.00 22.92 45 ATOM 1661 N LEU 424 7.103 10.773 67.309 1.00 22.78 ATOM 1662 CA LEU 424 7.512 11.306 65.936 1.00 23.40 ATOM 1663 CB LEU 424 8.405 12.531 65.875 1.00 24.54 ATOM 1664 CG LEU 424 9.777 12.226 66.517 1.00 22.52 ATOM 1665 CD1 LEU 424 8.589 12.892 64.405 1.00 22.78 50 ATOM 1666 CD2 LEU 424 6.422 11.861 68.153 1.00 22.46 ATOM 1667 C LEU 424 7.036 12.468 69.038 1.00 21.68 ATOM 1668 O LEU 424 5.136 12.101 67.900 1.00 22.38 ATOM 1669 N ARG 425 4.386 13.095 68.663 1.00 23.67 ATOM 1670 CA ARG 425 2.969 13.240 68.087 1.00 26.56 55 ATOM 1671 CB ARG 425 2.066 14.140 68.903 1.00 30.90 ATOM 1672 CG ARG 425 0.977 14.732 68.031 1.00 36.25 ATOM 1673 CD ARG 425





	ATOM		0.469 13.774 67.044 1.00 40.86	
	ATOM	1675 CZ ARG 425	-0.070 12.592 67.339 1.00 42.76	
	ATOM	1676 NH1 ARG 425	-0.183 12.196 68.604 1.00 46.63	
~	MOTA		-0.498 11.800 66.367 1.00 44.97	
5	ATOM	1678 C ARG 425	4.309 12.737 70.150 1.00 21.12	
	MOTA	1679 O ARG 425	4.418 13.604 71.021 1.00 21.30	
	ATOM	1680 N SER 426	4.124 11.452 70.436 1.00 19.60	
	ATOM	1681 CA SER 426	4.021 10.989 71.820 1.00 19.49	
10	ATOM	1682 CB SER 426		
10	ATOM	1683 OG SER 426	3.491 9.086 73.198 1.00 23.17	
	ATOM	1684 C SER 426	5.374 11.096 72.535 1.00 17.38	
	ATOM	1685 O SER 426	5.458 11.496 73.698 1.00 18.97	
	ATOM	1686 N ILE 427	6.419 10.742 71.812 1.00 18.11	
1.5	ATOM		7.770 10.812 72.368 1.00 15.88	
15	ATOM		8.763 10.095 71.449 1.00 15.75 10.213 10.351 71.913 1.00 17.78	
	ATOM	1689 CG2 ILE 427	8.479 8.591 71.526 1.00 17.78	
	MOTA	1690 CG1 ILE 427 1691 CD1 ILE 427	9.082 7.789 70.440 1.00 20.33	
	ATOM	1692 C ILE 427	8.146 12.272 72.599 1.00 16.69	
20	ATOM	1693 O ILE 427	8.779 12.589 73.606 1.00 16.41	
20	MOTA	1694 N SER 428	7.767 13.159 71.685 1.00 17.02	
	ATOM ATOM	1695 CA SER 428	8.059 14.590 71.884 1.00 17.37	
	ATOM	1696 CB SER 428		
	ATOM	1697 OG SER 428	7.745 16.794 70.876 1.00 19.14	
25	ATOM	1698 C SER 428	7.377 15.138 73.154 1.00 18.08	
23	ATOM	1699 O SER 428	7.968 15.916 73.928 1.00 16.98	
	ATOM	1700 N LEU 429	6.134 14.741 73.425 1.00 18.84	
	ATOM	1701 CA LEU 429		
	ATOM	1702 CB LEU 429	4.054 14.807 74.723 1.00 22.17	
30	ATOM	1703 CG LEU 429	3.187 15.432 73.625 1.00 25.96	
	MOTA	1704 CD1 LEU 429	1.800 14.809 73.624 1.00 28.92	
	ATOM	1705 CD2 LEU 429	3.087 16.943 73.855 1.00 29.57	
	ATOM	1706 C LEU 429	6.296 14.782 75.860 1.00 17.99	
	ATOM	1707 O LEU 429	6.465 15.527 76.816 1.00 18.52	
35	ATOM	1708 N LYS 430	6.778 13.544 75.830 1.00 18.39	
	ATOM	1709 CA LYS 430	7.540 13.047 76.957 1.00 17.66	
	ATOM	1710 CB LYS 430	7.780 11.544 76.826 1.00 19.73	
	MOTA	1711 CG LYS 430	8.539 10.975 78.020 1.00 23.74	
10	ATOM	1712 CD LYS 430	7.625 11.004 79.260 1.00 27.95 8.192 10.194 80.414 1.00 34.36	
40	MOTA	1713 CE LYS 430	7.167 10.122 81.490 1.00 36.64	
	MOTA	1714 NZ LYS 430	8.865 13.795 77.077 1.00 18.37	
	MOTA	1715 C LYS 430 1716 O LYS 430	9.346 14.034 78.191 1.00 18.47	
	ATOM ATOM	1716 O LYS 430 1717 N SER 431	9.435 14.174 75.936 0.50 17.09	AC1
45	ATOM	1718 CA SER 431	10,693 14.931 75.919 0.50 18.08	AC1
43	ATOM	1719 CB SER 431	11.102 15.238 74.471 0.50 17.50	AC1
	ATOM	1720 OG SER 431	12.180 16.159 74.413 0.50 19.63	AC1
	ATOM	1721 C SER 431	10.472 16.244 76.663 0.50 18.02	AC1
	ATOM	1722 O SER 431	11.297 16.668 77.464 0.50 17.75	AC1
50	ATOM	1723 N PHE 432	9.326 16.875 76.415 1.00 17.68	
	ATOM	1724 CA PHE 432	9.020 18.162 77.057 1.00 17.81	
	ATOM	1725 CB PHE 432	7.778 18.817 76.425 1.00 18.74	
	ATOM	1726 CG PHE 432	8.099 19.713 75.249 1.00 17.54	
	ATOM	1727 CD1 PHE 432	8.649 20.976 75.448 1.00 18.72	
55	ATOM	1728 CD2 PHE 432	7.851 19.290 73.958 1.00 17.78	
	ATOM	1729 CE1 PHE 432	8.941 21.800 74.351 1.00 18.20	
	ATOM	1730 CE2 PHE 432	8.135 20.093 72.863 1.00 18.04	
	MOTA	1731 CZ PHE 432	8.684 21.358 73.060 1.00 19.15	





	ATOM	1732 C PHE 432	8.817 17.989 78.550 1.00 18.32
	ATOM	1733 O PHE 432	9.170 18.872 79.330 1.00 20.66
	ATOM	1734 N GLU 433	8.249 16.852 78.964 1.00 17.15
	ATOM	1735 CA GLU 433	8.073 16.592 80.382 1.00 20.50
5	ATOM	1736 CB GLU 433	7.520 15.192 80.613 1.00 19.84
	ATOM	1737 CG GLU 433	6.045 15.053 80.320 1.00 27.71
	ATOM	1738 CD GLU 433	5.533 13.688 80.744 1.00 31.07
	MOTA	1739 OE1 GLU 433	5.964 13.224 81.823 1.00 34.98
	ATOM	1740 OE2 GLU 433	4.714 13.094 80.006 1.00 34.76
10	MOTA	1741 C GLU 433	9.437 16.691 81.052 1.00 19.32
	ATOM	1742 O GLU 433	9.574 17.322 82.106 1.00 20.27
	ATOM	1743 N HIS 434	10.438 16.059 80.435 1.00 18.45
	ATOM	1744 CA HIS 434	11.810 16.086 80.972 1.00 19.10
1.5	ATOM	1745 CB HIS 434	12.708 15.091 80.247 1.00 20.67
15	ATOM	1746 CG HIS 434	12.346 13.662 80.495 1.00 21.88
	ATOM	1747 CD2 HIS 434	12.196 12.621 79.642 1.00 22.64
	ATOM	1748 ND1 HIS 434	12.153 13.151 81.763 1.00 24.64
	MOTA	1749 CE1 HIS 434	11.901 11.857 81.678 1.00 26.38
20	ATOM ATOM	1750 NE2 HIS 434 1751 C HIS 434	11.924 11.509 80.403 1.00 25.49 12.448 17.471 80.900 1.00 19.47
20	ATOM	1751 C HIS 434 1752 O HIS 434	13.029 17.930 81.868 1.00 20.51
	ATOM	1753 N LEU 435	12.360 18.122 79.749 1.00 17.30
	ATOM	1754 CA LEU 435	12.926 19.464 79.614 1.00 17.70
	ATOM	1755 CB LEU 435	12.660 20.017 78.219 1.00 17.54
25	ATOM	1756 CG LEU 435	13.350 19.239 77.100 1.00 17.06
20	ATOM	1757 CD1 LEU 435	12.933 19.793 75.764 1.00 19.34
	ATOM	1758 CD2 LEU 435	14.874 19.343 77.242 1.00 19.09
	ATOM	1759 C LEU 435	12.334 20.411 80.653 1.00 17.96
	ATOM	1760 O LEU 435	13.034 21.260 81.193 1.00 18.73
30	ATOM	1761 N PHE 436	11.035 20.302 80.921 1.00 17.35
	ATOM	1762 CA PHE 436	10.460 21.192 81.936 1.00 18.85
	ATOM	1763 CB PHE 436	8.920 21.188 81.897 1.00 19.91
	ATOM	1764 CG PHE 436	8.340 21.916 80.720 1.00 22.43
	ATOM	1765 CD1 PHE 436	8.885 23.113 80.288 1.00 23.77
35	ATOM	1766 CD2 PHE 436	7.243 21.399 80.040 1.00 23.20
	ATOM	1767 CE1 PHE 436	8.353 23.783 79.202 1.00 25.60
	ATOM	1768 CE2 PHE 436	6.703 22.063 78.942 1.00 22.41
	ATOM	1769 CZ PHE 436	7.250 23.249 78.521 1.00 26.06
40	ATOM	1770 C PHE 436	10.916 20.802 83.332 1.00 20.10
40	ATOM ATOM	1771 O PHE 436 1772 N PHE 437	11.195 21.670 84.161 1.00 22.89 11.001 19.500 83.605 1.00 19.98
	ATOM	1773 CA PHE 437	11.412 19.023 84.922 1.00 21.11
	ATOM	1774 CB PHE 437	11.364 17.484 84.974 1.00 21.57
	ATOM	1775 CG PHE 437	11.628 16.913 86.339 1.00 25.91
45	ATOM	1776 CD1 PHE 437	10.633 16.924 87.313 1.00 27.17
	ATOM	1777 CD2 PHE 437	12.881 16.419 86.665 1.00 27.22
	ATOM	1778 CE1 PHE 437	10.891 16.447 88.599 1.00 30.66
	ATOM	1779 CE2 PHE 437	13.153 15.942 87.944 1.00 31.40
	ATOM	1780 CZ PHE 437	12.158 15.957 88.910 1.00 29.78
50	ATOM	1781 C PHE 437	12.807 19.496 85.305 1.00 22.67
	ATOM	1782 O PHE 437	13.046 19.895 86.464 1.00 24.17
	ATOM	1783 N PHE 438	13.724 19.453 84.346 1.00 19.58
	ATOM	1784 CA PHE 438	15.103 19.888 84.567 1.00 22.15
. .	ATOM	1785 CB PHE 438	16.038 19.027 83.718 1.00 22.90
55	ATOM	1786 CG PHE 438	16.093 17.595 84.171 1.00 23.82
	ATOM	1787 CD1 PHE 438	16.725 17.262 85.361 1.00 24.00
	ATOM	1788 CD2 PHE 438	15.509 16.584 83.419 1.00 27.39
	ATOM	1789 CE1 PHE 438	16.773 15.942 85.795 1.00 25.11





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	ATOM	1791 CZ PHE 438 1792 C PHE 438	15.334 21.383 84.256 1.00 21.04
	ATOM ATOM	1792 C PHE 438 1793 O PHE 438	16.454 21.875 84.352 1.00 22.98
5	ATOM		14.267 22.077 83.867 1.00 19.84
,	ATOM	1795 CA HIS 439	14.311 23.503 83.508 1.00 19.79
	ATOM	1796 CB HIS 439	14.550 24.380 84.742 1.00 21.68
	ATOM	1797 CG HIS 439	13.463 24.294 85.763 1.00 24.96
	ATOM	1798 CD2 HIS 439	12.345 25.037 85.939 1.00 27.66
10	ATOM	1799 ND1 HIS 439	13.440 23.331 86.747 1.00 26.44
	ATOM	1800 CE1 HIS 439	12.353 23.481 87.481 1.00 27.37
	ATOM	1801 NE2 HIS 439	11.672 24.511 87.012 1.00 28.08
	ATOM		15.375 23.803 82.469 1.00 20.93
	ATOM		16.185 24.726 82.626 1.00 23.42
15	ATOM	1804 N LEU 440	15.318 23.068 81.366 1.00 16.51
	ATOM	1805 CA LEU 440	16.289 23.200 80.301 1.00 18.97 16.820 21.813 79.917 1.00 19.31
	MOTA	1806 CB LEU 440 1807 CG LEU 440	17.585 21.101 81.017 1.00 19.31
	MOTA MOTA	1808 CD1 LEU 440	17.920 19.672 80.567 1.00 24.43
20	ATOM	1809 CD2 LEU 440	18.839 21.874 81.341 1.00 21.97
20	ATOM	1810 C LEU 440	15.751 23.859 79.042 1.00 20.05
	ATOM	1811 O LEU 440	16.497 24.030 78.099 1.00 21.82
	ATOM	1812 N VAL 441	14.478 24.229 79.038 1.00 19.87
	ATOM	1813 CA VAL 441	13.879 24.814 77.833 1.00 21.84
25	ATOM	1814 CB VAL 441	12.795 23.830 77.247 1.00 22.63
	ATOM	1815 CG1 VAL 441	11.601 23.713 78.192 1.00 22.79
	ATOM	1816 CG2 VAL 441	12.365 24.276 75.855 1.00 24.87
	ATOM	1817 C VAL 441	13.306 26.224 78.045 1.00 22.01 12.587 26.478 79.009 1.00 20.37
20	MOTA	1818 O VAL 441 1819 N ALA 442	12.587 26.478 79.009 1.00 20.37 13.646 27.122 77.120 1.00 23.96
30	MOTA MOTA	1819 N ALA 442 1820 CA ALA 442	13.233 28.529 77.172 1.00 27.08
	ATOM	1821 CB ALA 442	14.246 29.393 76.392 1.00 28.21
	ATOM	1822 C ALA 442	11.846 28.718 76.591 1.00 28.96
	ATOM	1823 O ALA 442	11.655 29.494 75.658 1.00 30.12
35	ATOM	1824 N ASP 443	10.895 28.011 77.178 1.00 30.46
	MOTA	1825 CA ASP 443	9,493 27,994 76,764 1.00 31.83
	MOTA	1826 CB ASP 443	8.678 27.367 77.906 1.00 33.17
	ATOM	1827 CG ASP 443	7.208 27.218 77.581 1.00 34.98
	MOTA	1828 OD1 ASP 443	6.856 26.945 76.404 1.00 37.47
40	ATOM	1829 OD2 ASP 443	6.404 27.346 78.524 1.00 31.58 8.873 29.320 76.318 1.00 31.97
	MOTA	1830 C ASP 443 1831 O ASP 443	8.426 29.453 75.180 1.00 30.41
	MOTA MOTA	1831 O ASP 443 1832 N THR 444	8.854 30.304 77.205 1.00 32.53
	ATOM	1833 CA THR 444	8.236 31.586 76.891 1.00 32.98
45	ATOM	1834 CB THR 444	7.965 32.371 78.198 1.00 34.53
.5	ATOM	1835 OG1 THR 444	9.196 32.581 78.900 1.00 37.04
	ATOM	1836 CG2 THR 444	7.020 31.577 79.102 1.00 35.95
	ATOM	1837 C THR 444	8.981 32.486 75.901 1.00 32.99
	ATOM	1838 O THR 444	8.399 33.436 75.370 1.00 32.71
50	ATOM	1839 N SER 445	10.248 32.179 75.639 1.00 30.56
	ATOM	1840 CA SER 445	11.071 32.977 74.727 1.00 29.90
	ATOM	1841 CB SER 445 1842 OG SER 445	12.481 33.132 75.313 1.00 29.52 12.418 33.766 76.576 1.00 31.76
	MOTA	1842 OG SER 445 1843 C SER 445	12.418 33.766 76.576 1.00 31.76
55	ATOM ATOM	1844 O SER 445	11.580 33.153 72.387 1.00 28.30
55	ATOM	1845 N ILE 446	10.875 31.151 73.133 1.00 26.98
	ATOM	1846 CA ILE 446	11.010 30.511 71.840 1.00 25.95
	ATOM	1847 CB ILE 446	10.656 29.013 71.961 1.00 26.36

ATOM 1848 CG2 ILE 446

ATOM 1849 CG1 ILE 446

ATOM 1850 CD1 ILE 446

ATOM 1851 C ILE 446

ATOM 1852 O ILE 446

ATOM 1853 N ALA 447

ATOM 1854 CA ALA 447

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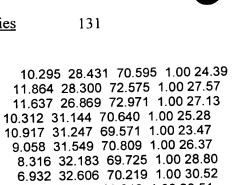
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ATOM 1855 CB ALA 447 ATOM 1856 C ALA 447 ATOM 1857 O ALA 447 10 ATOM 1858 N GLY 448 ATOM 1859 CA GLY 448

ATOM 1860 C GLY 448 ATOM 1861 O GLY 448 ATOM 1862 N TYR 449 ATOM 1863 CA TYR 449

ATOM 1864 CB TYR 449 ATOM 1865 CG TYR 449 ATOM 1866 CD1 TYR 449 ATOM 1867 CE1 TYR 449 ATOM 1868 CD2 TYR 449 ATOM 1869 CE2 TYR 449

ATOM 1870 CZ TYR 449 ATOM 1871 OH TYR 449 ATOM 1872 C TYR 449 25 ATOM 1873 O TYR 449 ATOM 1874 N ILE 450 ATOM 1875 CA ILE 450

ATOM 1876 CB ILE 450 ATOM 1877 CG2 ILE 450 30 ATOM 1878 CG1 ILE 450 ATOM 1879 CD1 ILE 450 ATOM 1880 C ILE 450 ATOM 1881 O ILE 450

ATOM 1882 N ARG 451 ATOM 1883 CA ARG 451 ATOM 1884 CB ARG 451 ATOM 1885 CG ARG 451 ATOM 1886 CD ARG 451 ATOM 1887 NE ARG 451

ATOM 1888 CZ ARG 451 ATOM 1889 NH1 ARG 451 ATOM 1891 C ARG 451 ATOM 1892 O ARG 451

ATOM 1893 N ASP 452 ATOM 1894 CA ASP 452 ATOM 1895 CB ASP 452 ATOM 1896 CG ASP 452 ATOM 1897 OD1 ASP 452 50

ATOM 1898 OD2 ASP 452 ATOM 1899 C ASP 452 ATOM 1900 O ASP 452 ATOM 1901 N ALA 453 ATOM 1902 CA ALA 453

ATOM 1903 CB ALA 453 ATOM 1904 C ALA 453 ATOM 1905 O ALA 453

9.114 33.394 69.218 1.00 28.51 9.229 33.608 68.005 1.00 29.41 9.675 34.164 70.155 1.00 28.53 10.474 35.337 69.811 1.00 27.89 11.762 34.993 69.095 1.00 28.77 12.167 35.692 68.162 1.00 28.23

12.435 33.927 69.536 1.00 27.26 13.666 33.502 68.872 1.00 28.14 14.262 32.267 69.553 1.00 26.16 14.683 32.492 70.990 1.00 28.82 14.913 33.782 71.482 1.00 29.84 15.336 33.988 72.802 1.00 32.66

14.881 31.412 71.853 1.00 29.90 15.306 31.604 73.173 1.00 30.71 15.532 32.887 73.641 1.00 32.74 15.979 33.070 74.939 1.00 36.98 13.361 33.150 67.420 1.00 27.51 14.116 33.491 66.513 1.00 27.99

12.254 32.442 67.207 1.00 27.41 11.876 32.053 65.861 1.00 27.70 10.662 31.102 65.863 1.00 26.64 10.292 30.744 64.413 1.00 26.88 11.003 29.846 66.690 1.00 27.46 9.811 28.956 67.032 1.00 24.45

11.534 33.295 65.041 1.00 29.34

11.994 33.440 63.911 1.00 30.32 10.735 34.187 65.617 1.00 30.43 10.351 35.416 64.923 1.00 33.00 9.514 36.306 65.851 1.00 32.56 8.874 37.519 65.161 1.00 34.91 7.955 38.328 66.076 1.00 36.14 6.768 37.599 66.518 1.00 37.46

6.669 36.943 67.672 1.00 40.02 6.669 36.943 67.672 1.00 40.02 7.690 36.921 68.521 1.00 41.16 ATOM 1890 NH2 ARG 451 5.547 36.299 67.976 1.00 40.59 11.629 36.138 64.472 1.00 34.57

11.761 36.516 63.298 1.00 34.59 12.578 36.304 65.392 1.00 36.05 13.837 36.975 65.070 1.00 39.88 14.690 37.184 66.331 1.00 42.41 14.004 38.065 67.364 1.00 46.01

13.162 38.897 66.961 1.00 46.57 14.315 37.934 68.576 1.00 48.55 14.657 36.212 64.039 1.00 40.80 15.219 36.805 63.112 1.00 42.52

14.730 34.896 64.197 1.00 41.16 15.493 34.071 63.272 1.00 42.41 15.585 32.643 63.796 1.00 41.71 14.904 34.070 61.863 1.00 44.06

15.635 33.910 60.887 1.00 44.96





	ATOM		13.590 34.259 61.759 1.00 45.34
	ATOM	1907 CA LEU 454	12.921 34.261 60,460 1.00 47.12
	ATOM	1908 CB LEU 454	11.419 33.989 60.631 1.00 42.61
	MOTA	1909 CG LEU 454	11.078 32.514 60.884 1.00 38.89
5	ATOM	1910 CD1 LEU 454	9.576 32.329 60.950 1.00 36.29
	ATOM	1911 CD2 LEU 454	11.660 31.657 59.764 1.00 36.23
	ATOM	1912 C LEU 454	13.149 35.544 59.669 1.00 50.37
	ATOM	1913 O LEU 454	13.255 35.506 58.443 1.00 51.61
10	ATOM	1914 N ARG 455	13.218 36.679 60.360 1.00 54.48
10	ATOM	1915 CA ARG 455	13.486 37.951 59.688 1.00 58.31
	ATOM	1916 CB ARG 455	13.128 39.147 60.582 1.00 59.22
	ATOM	1917 CG ARG 455	11.635 39.352 60.806 1.00 60.97
	ATOM	1918 CD ARG 455	11.318 40.787 61.228 1.00 62.50
1.5	MOTA	1919 NE ARG 455	10.998 40.919 62.648 1.00 64.04
15	MOTA	1920 CZ ARG 455	11.873 40.784 63.640 1.00 64.71 13.146 40.511 63.378 1.00 64.92
	MOTA MOTA	1921 NH1 ARG 455 1922 NH2 ARG 455	11.470 40.923 64.897 1.00 64.48
	ATOM	1923 C ARG 455	14.988 37.938 59.452 1.00 60.72
	ATOM	1924 O ARG 455	15.597 38.964 59.147 1.00 61.55
20	ATOM	1925 N ASN 456	15.557 36.743 59.597 1.00 63.01
20	ATOM	1926 CA ASN 456	16.983 36.482 59.463 1.00 64.82
	ATOM	1927 CB ASN 456	17.434 36.512 57.987 1.00 66.21
	ATOM	1928 CG ASN 456	17.254 37.871 57.327 1.00 67.51
	ATOM	1929 OD1 ASN 456	17.901 38.850 57.702 1.00 68.69
25	ATOM	1930 ND2 ASN 456	16.377 37.930 56.326 1.00 68.01
	ATOM	1931 C ASN 456	17.795 37.442 60.317 1.00 65.37
	MOTA	1932 O ASN 456	17.456 37.680 61.480 1.00 65.63
	MOTA	1933 N GLY 457	18.858 37.997 59.749 1.00 65.99
	ATOM	1934 CA GLY 457	19.704 38.896 60.510 1.00 66.46
30	ATOM	1935 C GLY 457	20.739 38.015 61.176 1.00 66.78
	ATOM	1936 O GLY 457	21.568 38.471 61.968 1.00 67.21
	MOTA	1937 N GLY 458	20.669 36.728 60.844 1.00 66.86
	MOTA	1938 CA GLY 458	21.594 35.753 61.384 1.00 66.84 22.018 34.761 60.315 1.00 66.86
35	ATOM ATOM	1939 C GLY 458 1940 O GLY 458	21.450 34.801 59.199 1.00 66.65
33	ATOM	1941 OXT GLY 458	22.922 33.943 60.593 1.00 65.49
	ATOM	1942 OH2 TIP 1003	30.252 23.128 74.386 1.00 27.69
	ATOM	1943 OH2 TIP 1005	14.203 25.558 89.644 1.00 25.22
	ATOM	1944 OH2 TIP 1006	8.388 25.042 72.262 1.00 22.81
40	ATOM	1945 OH2 TIP 1008	8.367 21.538 69.460 1.00 19.23
	ATOM	1946 OH2 TIP 1009	-7.350 22.030 52.884 1.00 80.11
	ATOM	1947 OH2 TIP 1010	-4.017 19.644 67.897 1.00 33.26
	MOTA	1948 OH2 TIP 1011	8.365 3.022 77.974 1.00 47.93
	MOTA	1949 OH2 TIP 1012	30.690 8.779 67.839 1.00 26.30
45	MOTA	1950 OH2 TIP 1013	12.264 8.843 80.249 1.00 26.01
	ATOM	1951 OH2 TIP 1014	-1.764 16.382 62.652 1.00 44.82
	ATOM	1952 OH2 TIP 1015	20.301 34.946 75.498 1.00 51.92
	ATOM	1953 OH2 TIP 1016	14.443 15.693 61.296 1.00 22.04
50	ATOM	1954 OH2 TIP 1017	12.487 31.635 78.951 1.00 36.76
50	ATOM	1955 OH2 TIP 1018	16.579 6.557 83.739 1.00 27.86
	MOTA	1956 OH2 TIP 1019 1957 OH2 TIP 1021	-0.626 26.615 50.499 1.00 30.82 3.543 20.127 64.859 1.00 23.80
	MOTA	1957 OH2 TIP 1021 1958 OH2 TIP 1022	4.772 0.996 47.855 1.00 40.67
	MOTA MOTA	1959 OH2 TIP 1023	9.799 29.451 51.621 1.00 30.93
55	ATOM	1960 OH2 TIP 1024	7.476 19.030 68.589 1.00 22.30
55	ATOM	1961 OH2 TIP 1025	20.355 7.131 58.551 1.00 52.44
	ATOM	1962 OH2 TIP 1026	-0.829 29.526 57.153 1.00 31.90
	ATOM	1963 OH2 TIP 1027	11.560 -6.342 53.442 1.00 52.29





	ATOM	1964 OH2 TIP	1028	15.278 0.625 72.808 1.00 27.12
	ATOM	1965 OH2 TIP	1029	22.593 26.832 76.012 1.00 35.56
	ATOM	1966 OH2 TIP	1031	3.001 25.878 68.078 1.00 22.76
	MOTA	1967 OH2 TIP	1032	13.489 25.800 47.958 1.00 47.50
5	ATOM	1968 OH2 TIP	1033	-7.554 18.088 60.905 1.00 30.53
	ATOM	1969 OH2 TIP	1034	24.742 18.595 64.446 1.00 44.88
	ATOM	1970 OH2 TIP	1035	13.751 37.059 78.800 1.00 60.77
	ATOM	1971 OH2 TIP	1036	-0.515 10.167 75.163 1.00 36.51
	ATOM	1972 OH2 TIP	1037	12.373 35.911 72.901 1.00 32.65
10	ATOM	1973 OH2 TIP	1039	23.543 26.270 78.523 1.00 24.40
	MOTA	1974 OH2 TIP	1040	17.896 20.961 59.259 1.00 39.57
	MOTA	1975 OH2 TIP	1041	8.248 15.187 89.930 1.00 59.85
	ATOM	1976 OH2 TIP	1042	7.418 31.128 73.133 1.00 34.33
	ATOM		1043	21.123 8.890 53.894 1.00 67.39
15	MOTA	1978 OH2 TIP	1045	15.162 18.243 53.355 1.00 28.26
	MOTA	1979 OH2 TIP	1050	4.216 23.224 44.827 1.00 46.56
	ATOM		1051	17.523 1.262 73.909 1.00 23.12
	ATOM		1052	-0.169 20.149 67.166 1.00 67.45
	ATOM		1053	20.135 12.837 55.866 1.00 51.70
20	MOTA	1983 OH2 TIP	1054	10.612 35.387 77.215 1.00 57.20
	ATOM	1984 OH2 TIP	1055	14.587 38.805 73.912 1.00 56.14
	MOTA	1985 OH2 TIP	1056	22.658 15.094 55.769 1.00 63.46
	MOTA		1057	8.196 1.415 39.058 1.00 55.65
	ATOM	1987 OH2 TIP	1058	10.807 2.725 77.173 1.00 22.15
25	ATOM		1059	19.013 20.604 62.130 1.00 32.43
	ATOM		1061	2.388 16.861 45.084 1.00 25.70
	ATOM	1990 OH2 TIP	1063	5.229 6.816 86.424 1.00 59.99
	ATOM		1501	18.919 15.965 66.146 1.00 24.36
20	ATOM		1502	2.744 33.258 66.246 1.00 30.10
30	ATOM		1503	4.527 17.244 77.877 1.00 23.98
	ATOM	1994 OH2 TIP	1504	-0.815 22.723 68.903 1.00 24.06
	ATOM	1995 OH2 TIP	1506	22.697 1.204 69.760 1.00 28.71 12.438 25.185 81.547 1.00 28.20
	MOTA		1507 1508	12.438 25.185 81.547 1.00 28.20 17.107 31.275 76.636 1.00 33.34
35	ATOM ATOM		1509	17.107 31.273 70.030 1.00 33.34
33	ATOM	1998 OH2 TIP	1510	7.197 12.183 44.002 1.00 29.62
	ATOM	2000 OH2 TIP	1511	-4.834 15.832 60.463 1.00 33.76
	ATOM		1512	11.093 1.186 74.736 1.00 29.08
	ATOM		1513	-0.145 2.568 51.845 1.00 30.78
40	ATOM		1514	-6.100 23.488 73.541 1.00 27.96
10	ATOM		1515	8.298 14.512 44.198 1.00 34.89
	ATOM	2005 OH2 TIP		0.418 26.098 68.989 1.00 28.71
	ATOM	2006 OH2 TIP		-7.177 16.116 59.030 1.00 32.04
	ATOM			18.000 18.387 62.314 1.00 32.49
45	ATOM	2008 OH2 TIP		21.777 20.403 61.898 1.00 38.66
	ATOM		1521	-1.379 32.714 63.883 1.00 40.86
	ATOM		1522	1.931 22.610 68.721 1.00 31.49
	ATOM		1523	-3.158 9.157 64.790 1.00 46.08
	ATOM	2012 OH2 TIP	1524	2.081 4.709 65.432 1.00 38.87
50	ATOM	2013 OH2 TIP	1525	3.829 11.325 75.940 1.00 34.36
	ATOM	2014 OH2 TIP	1527	21.845 33.747 71.839 1.00 51.86
	MOTA	2015 OH2 TIP	1528	12.196 0.941 78.760 1.00 46.53
	MOTA		1529	30.316 21.478 85.009 1.00 28.49
	ATOM	2017 OH2 TIP	1530	9,786 2,798 91,182 1,00 58,36
55	MOTA	2018 OH2 TIP	1531	16.571 8.007 48.772 1.00 38.32
	MOTA	2019 OH2 TIP	1532	3.764 24.595 70.409 1.00 31.40
	ATOM		1533	-0.952 5.111 57.996 1.00 39.42
	ATOM	2021 OH2 TIP	1534	8.395 29.793 48.733 1.00 45.92



	ATOM	2022 OH2 TIP	1535	18.190 -0.943 54.382 1.00 55.57
	ATOM		1536	4.583 13.859 64.203 1.00 30.44
	ATOM		1538	12.012 14.232 84.365 1.00 33.97
	ATOM		1539	-1.284 36.017 69.736 1.00 57.91
5	ATOM		1540	2.454 15.898 79.022 1.00 40.22
-	ATOM		1544	2.719 2.670 49.088 1.00 32.00
	ATOM	2028 OH2 TIP	1545	13.537 37.410 71.136 1.00 41.29
	ATOM	2029 OH2 TIP	1546	22.697 0.071 79.248 1.00 32.01
	ATOM	2030 OH2 TIP	1548	-0.239 7.542 39.851 1.00 52.37
10	MOTA	2031 OH2 TIP	1549	0.076 10.603 44.453 1.00 41.67
	ATOM		1550	31.157 3.039 59.611 1.00 43.66
	ATOM		1551	4.226 34.045 72.549 1.00 53.58
	ATOM		1554	10.022 33.359 56.088 1.00 41.48
	MOTA		1555	-1.058 37.708 61.917 1.00 54.81
15	ATOM		1556	-4.583 15.870 53.480 1.00 37.02
	ATOM		1557	23.851 8.517 92.595 1.00 36.91
	ATOM		1558	-7.204 28.744 59.955 1.00 35.72
	ATOM		1560	19.483 16.334 88.331 1.00 34.61
20	ATOM		1561	1.968 8.086 38.648 1.00 57.90
20	ATOM		1562	32.430 -4.459 71.625 1.00 63.22
	MOTA		1563	7.819 12.682 83.368 1.00 47.71 -5.435 18.376 72.810 1.00 41.90
	MOTA		1564	-5.435 18.376 72.810 1.00 41.90 19.550 17.394 63.917 1.00 31.79
	ATOM ATOM		1565 1566	24.069 28.502 85.703 1.00 50.24
25	ATOM		1568	26.854 12.830 56.392 1.00 51.68
23	ATOM		1570	3.595 32.325 68.760 1.00 45.07
	ATOM		1571	24.805 8.300 62.036 1.00 28.27
	ATOM		1572	4.194 17.554 63.640 1.00 26.21
	ATOM		1573	2.589 20.195 67.352 1.00 34.52
30	ATOM		1574	15.713 17.937 61.017 1.00 52.03
	ATOM		1575	-9.321 14.210 59.772 1.00 33.92
	ATOM		1576	13.215 7.332 82.542 1.00 31.45
	ATOM	2054 OH2 TIP	1577	10.470 24.539 83.194 1.00 35.29
	ATOM	2055 OH2 TIP	1578	25.712 17.999 53.496 1.00 41.46
35	ATOM		1579	9.445 -0.239 41.882 1.00 41.51
	MOTA		1580	6.603 16.005 42.611 1.00 32.35
	ATOM		1581	-1.523 7.654 59.739 1.00 50.11
	ATOM		1582	8.397 34.515 72.891 1.00 33.81
	ATOM		1583	2.742 39.191 60.949 1.00 39.77
40	ATOM		1584	18.933 6.009 52.002 1.00 45.27
	ATOM		1585	-1.653 20.171 69.665 1.00 37.15
	ATOM	_ •	1586	-2.633 4.655 52.475 1.00 49.05
	ATOM	2064 OH2 TIP		36.297 28.180 83.444 1.00 41.56
15	MOTA		1588	-0.851 31.806 55.808 1.00 34.41
45	MOTA		1589	4.002 34.625 70.007 1.00 46.13 32.711 20.152 84.581 1.00 53.56
	MOTA		1590 1591	
	ATOM ATOM		1593	19.998 6.099 87.630 1.00 31.12 -0.189 3.637 35.682 1.00 54.58
	ATOM		1594	12.455 12.705 39.358 1.00 55.12
50	ATOM		1596	-2.554 -6.074 47.925 1.00 55.01
50	ATOM		1597	5.017 28.176 75.017 1.00 42.02
	ATOM		1598	28.617 32.433 80.891 1.00 65.40
	ATOM		1599	8.680 7.258 78.481 1.00 52.56
	ATOM		1600	18.188 12.950 87.437 1.00 47.03
55	ATOM			-11.532 19.931 55.756 1.00 48.92
	ATOM		1602	22.073 14.215 52.571 1.00 49.32
	ATOM	2078 OH2 TIP		-3.860 34.262 53.170 1.00 48.97
	MOTA		1604	1.118 10.847 82.180 1.00 44.11





ATOM 2080 OH2 TIP 1605 19.335 32.031 77.782 1.00 48.61 ATOM 2081 OH2 TIP 1606 19.174 9.955 48.654 1.00 40.42 ATOM 2082 OH2 TIP 1607 23.632 -1.631 71.300 1.00 37.97 ATOM 2083 OH2 TIP 1608 26.622 26.695 85.361 1.00 44.14 ATOM 2084 OH2 TIP 1609 22.586 -1.769 57.526 1.00 48.15 ATOM 2084 OH2 TIP 1609
ATOM 2085 OH2 TIP 1610
ATOM 2086 OH2 TIP 1611
ATOM 2086 OH2 TIP 1611
ATOM 2087 OH2 TIP 1612
ATOM 2088 OH2 TIP 1614
ATOM 2089 OH2 TIP 1615
ATOM 2090 OH2 TIP 1616
ATOM 2091 OH2 TIP 1618
ATOM 2092 OH2 TIP 1619
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ATOM 2097 OH2 TIP 1621
ATOM 2098 OH2 TIP 1619
ATOM 2098 OH2 TIP 1619 10 ATOM 2094 OH2 TIP 1622 3.271 9.154 86.392 1.00 55.17 ATOM 2095 OH2 TIP 1627 3.433 19.409 44.225 1.00 50.54 ATOM 2096 OH2 TIP 1628 2.390 26.629 72.360 1.00 42.60 15 ATOM 2097 OH2 TIP 1629 9.893 39.104 69.833 1.00 54.40 ATOM 2098 OH2 TIP 1630 2.709 14.153 43.455 1.00 34.37 ATOM 2099 OH2 TIP 1631 11.049 12.448 88.232 1.00 45.81 20 ATOM 2100 OH2 TIP 1632 4.576 31.506 72.757 1.00 39.34 ATOM 2101 OH2 TIP 1634 6.784 36.285 71.148 1.00 51.53 ATOM 2102 OH2 TIP 1635 6.667 43.335 56.568 1.00 51.21 ATOM 2103 OH2 TIP 1636 -5.771 9.260 60.442 1.00 44.79 25 ATOM 2104 OH2 TIP 1638 0.052 33.418 66.937 1.00 47.03 ATOM 2105 OH2 TIP 1641 0.354 1.055 46.133 1.00 54.03 ATOM 2106 OH2 TIP 1642 24.406 30.113 88.300 1.00 48.82 26.619 20.182 66.495 1.00 38.01 ATOM 2107 OH2 TIP 1643 ATOM 2108 OH2 TIP 1644 17.492 7.024 42.815 1.00 65.02 30 ATOM 2109 OH2 TIP 1645 25.942 26.481 82.676 1.00 49.52 ATOM 2110 OH2 TIP 1646 20,601 16.199 68.672 1.00 37.35 27.616 9.156 63.460 1.00 37.92 ATOM 2111 OH2 TIP 1649 0.428 -3.038 44.190 1.00 54.50 ATOM 2112 OH2 TIP 1650 ATOM 2113 OH2 TIP 1652 -7.028 20.462 59.299 1.00 33.58 -2.848 32.314 67.354 1.00 49.02 -0.686 17.762 66.362 1.00 46.03 19.583 17.275 60.162 1.00 41.00 35 ATOM 2114 OH2 TIP 1653 ATOM 2115 OH2 TIP 1654 ATOM 2116 OH2 TIP 1655 13.719 36.618 75.139 1.00 51.89 ATOM 2117 OH2 TIP 1656 9.386 -0.422 71.399 1.00 43.15 ATOM 2118 OH2 TIP 1657 40 ATOM 2119 OH2 TIP 1659 23.690 28.880 79.578 1.00 42.62 ATOM 2120 OH2 TIP 1660 22.069 3.800 58.682 1.00 46.06 ATOM 2121 OH2 TIP 1661 20.671 13.353 58.841 1.00 57.05 27.473 10.135 82.332 1.00 47.43 ATOM 2122 OH2 TIP 1662 ATOM 2123 OH2 TIP 1664 9.564 26.542 84.601 1.00 44.55 ATOM 2124 OH2 TIP 1666 29.122 9.606 65.764 1.00 45.20 45 ATOM 2125 OH2 TIP 1668 13.135 20.507 41.865 1.00 59.09 ATOM 2126 OH2 TIP 1669 22.639 11.672 58.999 1.00 54.98 ATOM 2127 OH2 TIP 1670 -1.845 6.027 76.197 1.00 48.89 ATOM 2128 OH2 TIP 1672 4.883 25.252 42.734 1.00 51.13 ATOM 2129 OH2 TIP 1675 1.329 39.322 66.763 1.00 68.30 50 ATOM 2130 OH2 TIP 1676 12.783 29.313 87.079 1.00 54.62 ATOM 2131 OH2 TIP 1679 25.035 18.339 57.364 1.00 54.53 ATOM 2132 OH2 TIP 1682 29.392 -1.856 57.721 1.00 37.30 ATOM 2133 OH2 TIP 1683 28.780 9.970 58.622 1.00 54.22 ATOM 2134 OH2 TIP 1685 4.741 39.274 62.499 1.00 46.58 55 ATOM 2135 OH2 TIP 1686 -3.084 6.977 49.478 1.00 57.17 ATOM 2136 OH2 TIP 1687 26.519 30.868 83.197 1.00 64.53 -2.784 37.278 67.289 1.00 59.53 ATOM 2137 OH2 TIP 1688



	ATOM 2429 OU2 TID 4690	10.604 10.604 80.206 1.00.52.44
	ATOM 2138 OH2 TIP 1689	18.691 10.604 88.296 1.00 52.44
	ATOM 2139 OH2 TIP 1690	27.919 6.703 82.226 1.00 44.84
	ATOM 2140 OH2 TIP 1691	-4.338 11.103 48.033 1.00 55.91
_	ATOM 2141 OH2 TIP 1692	-7.853 9.429 46.864 1.00 63.74
5	ATOM 2142 OH2 TIP 1693	10.901 -1.686 67.477 1.00 41.21
	ATOM 2143 OH2 TIP 1694	-2.114 6.315 55.259 1.00 56.21
	ATOM 2144 OH2 TIP 1695	17.482 15.932 44.391 1.00 41.18
	ATOM 2145 OH2 TIP 1696	-12.326 38.088 61.786 1.00 53.30
	ATOM 2146 OH2 TIP 1697	-2.176 40.471 68.230 1.00 68.88
10	ATOM 2147 OH2 TIP 1700	6.514 -1.974 53.366 1.00 51.67
	ATOM 2148 OH2 TIP 1701	21.800 10.610 55.773 1.00 60.93
	ATOM 2149 OH2 TIP 1702	3.975 27.046 41.446 1.00 44.88
	ATOM 2150 OH2 TIP 1703	26.678 -3.660 64.081 1.00 62.42
	ATOM 2151 OH2 TIP 1704	2.958 12.027 86.133 1.00 53.52
15	ATOM 2151 OH2 TIP 1704 ATOM 2152 OH2 TIP 1705	4.264 22.050 63.018 1.00 16.96
13		
	ATOM 2153 OH2 TIP 1706	22.999 26.329 63.006 1.00 32.17
	ATOM 2154 OH2 TIP 1707	5.614 2.688 68.201 1.00 42.08
	ATOM 2155 OH2 TIP 1708	-2.967 17.730 54.394 1.00 38.89
• •	ATOM 2156 OH2 TIP 1709	25.853 10.594 62.118 1.00 43.50
20	ATOM 2157 OH2 TIP 1711	13.060 12.966 86.563 1.00 41.22
	ATOM 2158 OH2 TIP 1712	19.784 15.472 45.489 1.00 58.17
	ATOM 2159 OH2 TIP 1713	10.567 14.806 42.991 1.00 43.48
	ATOM 2160 OH2 TIP 1714	24.079 30.190 83.477 1.00 47.61
	ATOM 2161 OH2 TIP 1715	23.927 21.975 63.464 1.00 44.77
25	ATOM 2162 OH2 TIP 1716	15.801 20.193 58.769 1.00 34.32
	ATOM 2163 OH2 TIP 1717	23.867 27.717 72.712 1.00 40.47
	ATOM 2164 OH2 TIP 1718	24.567 27.201 69.884 1.00 45.97
	ATOM 2165 OH2 TIP 1719	32.141 -1.375 73.278 1.00 62.31
	ATOM 2166 OH2 TIP 1720	19.799 24.122 57.454 1.00 35.07
30	ATOM 2167 OH2 TIP 1721	18.297 23.286 53.598 1.00 43.88
50	ATOM 2168 OH2 TIP 1722	8.617 1.105 73.470 1.00 48.55
		28.598 25.728 64.296 1.00 46.24
		19.225 33.547 73.276 1.00 44.07
	ATOM 2170 OH2 TIP 1725	
25	ATOM 2171 OH2 TIP 1726	1.762 4.546 47.584 1.00 50.27
35	ATOM 2172 OH2 TIP 1727	10.895 28.774 83.657 1.00 54.87
	ATOM 2173 OH2 TIP 1728	9.989 36.628 73.713 1.00 46.56
	ATOM 2174 OH2 TIP 1729	-1.331 8.332 70.133 1.00 46.76
	ATOM 2175 OH2 TIP 1730	24.262 12.802 55.386 1.00 59.24
	ATOM 2176 OH2 TIP 1731	28.623 25.788 86.798 1.00 51.87
40	ATOM 2177 OH2 TIP 1732	-0.501 4.843 68.521 1.00 47.96
	ATOM 2178 OH2 TIP 1736	18.422 4.635 54.793 1.00 51.00
	ATOM 2179 OH2 TIP 1737	-5.388 27.319 50.727 1.00 46.53
	ATOM 2180 OH2 TIP 1738	-2.286 20.842 72.915 1.00 45.95
	ATOM 2181 OH2 TIP 1739	0.996 4.268 39.511 1.00 52.67
45	ATOM 2182 OH2 TIP 1740	-10.886 28.616 64.116 1.00 45.22
	ATOM 2183 OH2 TIP 1741	20.353 -4.883 70.512 1.00 61.31
	ATOM 2184 OH2 TIP 1742	22.491 16.164 60.365 1.00 58.19
	ATOM 2185 OH2 TIP 3001	15.272 21.419 87.789 1.00 27.44
	ATOM 2186 OH2 TIP 3002	13.055 32.876 52.925 1.00 53.35
50	ATOM 2187 OH2 TIP 3006	16.014 18.841 64.083 1.00 56.45
50		16.802 30.100 54.388 1.00 48.87
		13.673 27.099 82.740 1.00 32.07
	ATOM 2189 OH2 TIP 3009	
	ATOM 2190 OH2 TIP 3010	30.041 24.325 84.969 1.00 41.40
~ ~	ATOM 2191 OH2 TIP 3007	-2.102 35.612 60.958 1.00 52.05
55	ATOM 2192 OH2 TIP 3011	7.242 14.501 40.017 1.00 51.46
	ATOM 2193 OH2 TIP 3012	1.031 36.834 60.593 1.00 49.05
	ATOM 2194 OH2 TIP 3013	0.026 24.244 72.355 1.00 42.35
	ATOM 2195 OH2 TIP 3015	-7.871 31.986 57.037 1.00 46.09





	ATOM	2196 OH2 TIP 3019	8.655 -3.490 62.423 1.00 44.56	
		2197 OH2 TIP 3020	-0.191 30.553 51.677 1.00 54.31	
	ATOM			
	MOTA	2198 OH2 TIP 3023	3.107 37.905 57.599 1.00 48.07	
_	ATOM	2199 OH2 TIP 3024	26.217 6.182 84.277 1.00 47.75	
5	ATOM	2200 OH2 TIP 3025	2.594 16.520 65.838 1.00 40.67	
	ATOM	2201 C1 EPH 4000	23.874 12.843 85.264 1.00 42.79	
	ATOM	2202 C2 EPH 4000	23.099 13.772 86.129 1.00 44.39	
	ATOM	2203 C4 EPH 4000	24.923 13.000 83.062 1.00 45.55	
	ATOM	2204 O2 EPH 4000	24.221 13.543 84.059 1.00 44.96	
10	ATOM	2205 O4 EPH 4000	25.350 11.876 83.028 1.00 47.53	
	ATOM	2206 C18 EPH 4000	25.126 14.045 81.931 1.00 47.05	
	ATOM	2207 C19 EPH 4000	24.674 13.569 80.547 1.00 46.98	
	ATOM	2208 C20 EPH 4000	23.168 13.412 80.473 1.00 49.00	
	ATOM	2209 C21 EPH 4000	22.772 12.939 79.111 1.00 51.06	
15		2210 C22 EPH 4000	21.365 12.327 79.073 1.00 52.88	
15	MOTA			
	ATOM	2211 C23 EPH 4000	20.291 13.230 78.423 1.00 54.24	
	ATOM	2212 C24 EPH 4000	20.651 13.777 77.022 1.00 55.08	
	MOTA	2213 C25 EPH 4000	19.987 15.129 76.704 1.00 56.13	
	ATOM	2214 C26 EPH 4000	20.807 16.375 77.147 1.00 56.19	
20	ATOM	2215 C27 EPH 4000	19.981 17.687 77.287 1.00 56.74	
	ATOM	2216 C28 EPH 4000	19.188 18.077 76.015 1.00 56.93	
	ATOM	2217 C29 EPH 4000	20.055 18.393 74.792 1.00 57.07	
	ATOM	2218 C30 EPH 4000	19.294 18.387 73.442 1.00 58.24	
	ATOM	2219 C31 EPH 4000	19.391 17.124 72.550 1.00 58.70	
25	ATOM	2220 C32 EPH 4000	18.019 16.479 72.198 1.00 59.07	
	ATOM	2221 C33 EPH 4000	16.762 17.158 72.768 1.00 59.61	
	ATOM	2222 C34 EPH 4000	15.463 16.541 72.231 1.00 60.17	
	ATOM	2223 C37 EPH 4000	22,780 13.059 87.421 1.00 47.03	
	ATOM	2224 O5 EPH 4000	22.047 13.939 88.273 1.00 53.23	
20		2225 P1 EPH 4000	21.699 13.222 89.578 1.00 56.71	
30	MOTA		20.350 13.536 89.939 1.00 58.07	
	ATOM	2226 O6 EPH 4000		
	MOTA	2227 O7 EPH 4000	22.579 12.360 90.311 1.00 56.72	
	MOTA	2228 O8 EPH 4000	22.167 14.340 90.336 1.00 55.93	
	ATOM	2229 C3 EPH 4000	21.561 15.394 85.253 1.00 42.20	
35	ATOM	2230 O1 EPH 4000	21.886 14.117 85.454 1.00 40.69	
	ATOM	2231 O3 EPH 4000	22.221 16.347 85.571 1.00 40.97	
	ATOM	2232 C5 EPH 4000	20.215 15.530 84.546 1.00 40.77	
	ATOM	2233 C6 EPH 4000	20.313 15.776 83.050 1.00 42.19	
	ATOM	2234 C7 EPH 4000	18.924 15.916 82.453 1.00 43.05	
40	ATOM	2235 C8 EPH 4000	18.900 15.944 80.947 1.00 44.57	
	ATOM	2236 C9 EPH 4000	17.477 16.101 80.445 1.00 45.49	
	ATOM	2237 C10 EPH 4000	17.167 15.209 79.273 1.00 47.18	
	MOTA	2238 C11 EPH 4000	16.561 15.987 78.117 1.00 47.85	
	ATOM	2239 C12 EPH 4000	15.158 15.514 77.781 1.00 49.75	
45	ATOM	2240 C13 EPH 4000	15.158 14.254 76.932 1.00 49.27	
15	ATOM	2241 C14 EPH 4000	14.899 14.563 75.454 1.00 51.41	
	ATOM	2242 C15 EPH 4000	14.958 13.341 74.490 1.00 51.93	
	ATOM	2243 C16 EPH 4000	16.376 12.870 74.074 1.00 52.39	
		2244 C17 EPH 4000	16.681 11.465 74.554 1.00 52.37	
50	MOTA		17.830 11.518 75.525 1.00 52.96	
50	ATOM	2245 C35 EPH 4000		
	ATOM	2246 C36 EPH 4000	17.968 10.168 76.193 1.00 53.00	
	ATOM	2247 C38 EPH 4000	22.197 10.885 90.057 1.00 56.75	
	MOTA	2248 C39 EPH 4000	23.458 10.026 89.911 1.00 56.42	
	ATOM	2249 N1 EPH 4000	24.546 10.825 89.334 1.00 54.45	
55	ATOM	2250 N SER 236	17.914 25.370 86.674 0.50 20.48	AC2
	ATOM	2251 CA SER 236	18.176 23.976 86.323 0.50 19.91	AC2
	ATOM	2252 CB SER 236	19.157 23.889 85.166 0.50 18.72	AC2
	ATOM	2253 OG SER 236	19.325 22.538 84.787 0.50 17.70	AC2



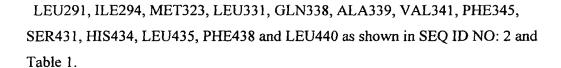


5 10	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2255 O SER 236 2256 N SER 247 2257 CA SER 247 2258 CB SER 247 2259 OG SER 247 2260 C SER 247 2261 O SER 247 2262 N SER 271 2263 CA SER 271 2264 CB SER 271 2265 OG SER 271 2266 C SER 271 2267 O SER 271 2268 N PRO 319	18.741 23.171 87.483 0.50 21.62 19.744 23.549 88.075 0.50 20.94 25.235 21.608 79.357 0.50 19.68 25.203 22.865 78.619 0.50 20.48 26.051 23.917 79.337 0.50 19.95 26.032 25.152 78.637 0.50 20.60 25.725 22.638 77.203 0.50 20.84 25.203 23.202 76.238 0.50 21.05 7.551 30.448 53.176 0.50 29.97 7.680 31.880 53.442 0.50 31.61 8.888 32.443 52.695 0.50 32.22 8.666 32.395 51.295 0.50 32.71 6.432 32.648 53.010 0.50 32.99 6.229 33.796 53.408 0.50 34.05 18.143 -4.099 74.681 0.50 41.20	AC2 AC2 AC2 AC2 AC2 AC2 AC2 AC2 AC2 AC2
20	ATOM ATOM ATOM ATOM ATOM	2269 CD PRO 319 2270 CA PRO 319 2271 CB PRO 319 2272 CG PRO 319 2273 C PRO 319 2274 O PRO 319	18.070 -4.311 76.139 0.50 40.63 18.053 -2.673 74.356 0.50 38.50 17.702 -2.038 75.699 0.50 39.26 18.406 -2.938 76.680 0.50 39.94 19.321 -2.077 73.756 0.50 35.96 20.410 -2.230 74.313 0.50 35.87	AC2 AC2 AC2 AC2 AC2 AC2
25	ATOM ATOM ATOM ATOM ATOM	2275 N GLN 343 2276 CA GLN 343 2277 CB GLN 343 2278 CG GLN 343 2279 CD GLN 343 2280 OE1 GLN 343	13.913 5.584 80.085 0.50 18.73 12.714 5.137 79.387 0.50 19.83 11.463 5.365 80.243 0.50 21.34 10.903 4.078 80.837 0.50 26.09 9.539 4.244 81.488 0.50 27.02 9.412 4.823 82.562 0.50 29.15	AC2 AC2 AC2 AC2 AC2 AC2
30	ATOM	2281 NE2 GLN 343	8.508 3.730 80.829 0.50 29.67	AC2
	ATOM	2282 C GLN 343	12.545 5.813 78.025 0.50 19.53	AC2
	ATOM	2283 O GLN 343	12.317 5.141 77.022 0.50 19.10	AC2
	ATOM	2284 N SER 353	14.027 4.461 65.783 0.50 19.97	AC2
	ATOM	2285 CA SER 353	15.191 3.950 65.107 0.50 20.43	AC2
	ATOM	2286 CB SER 353	16.391 4.058 66.033 0.50 20.57	AC2
35	ATOM	2287 OG SER 353	17.540 4.234 65.262 0.50 19.64	AC2
	ATOM	2288 C SER 353	15.054 2.524 64.574 0.50 21.08	AC2
	ATOM	2289 O SER 353	15.234 2.291 63.378 0.50 21.51	AC2
	ATOM	2290 N ARG 392	0.696 20.186 53.122 0.50 19.50	AC2
	ATOM	2291 CA ARG 392	0.935 18.822 53.549 0.50 19.96	AC2
40	ATOM ATOM ATOM ATOM ATOM	2292 CB ARG 392 2293 CG ARG 392 2294 CD ARG 392 2295 NE ARG 392 2296 CZ ARG 392	0.325 18.551 54.925 0.50 19.99 0.603 17.129 55.384 0.50 19.08 0.140 16.884 56.805 0.50 19.85 -1.315 16.885 56.925 0.50 19.23 -1.962 16.577 58.046 0.50 21.63	AC2 AC2 AC2 AC2 AC2
45	ATOM	2297 NH1 ARG 392	-1.283 16.242 59.138 0.50 19.92	AC2
	ATOM	2298 NH2 ARG 392	-3.289 16.611 58.086 0.50 22.19	AC2
	ATOM	2299 C ARG 392	0.338 17.878 52.501 0.50 19.95	AC2
	ATOM	2300 O ARG 392	0.940 16.867 52.149 0.50 20.64	AC2
	ATOM	2301 N SER 431	9.466 14.172 75.955 0.50 16.96	AC2
50	ATOM	2302 CA SER 431	10.735 14.900 76.047 0.50 17.25	AC2
	ATOM	2303 CB SER 431	11.346 15.109 74.659 0.50 17.09	AC2
	ATOM	2304 OG SER 431	10.765 16.211 73.998 0.50 16.93	AC2
	ATOM	2305 C SER 431	10.466 16.249 76.719 0.50 17.71	AC2
	ATOM	2306 O SER 431	11.267 16.716 77.521 0.50 17.14	AC2

6. A LBD according to Claim 5, comprising a ligand-binding pocket which is defined by the amino acids LEU230, VAL238, PRO239, PHE242, LEU249,

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- A LBD according to Claim 5, comprising a ligand-binding pocket which is defined by the amino acids LEU230, VAL238, PRO239, PHE242, PRO245, VAL246, LEU249, CYS250, GLY253, ASN287, LEU290, LEU291, ILE294, MET323, LEU325, LEU331, SER335, ALA336, GLN338, ALA339, VAL341, ILE344, PHE345, VAL348, SER431, HIS434, LEU435, PHE438, LEU440 as shown in SEQ ID NO: 2 and Table 1.
 - 8. A computer-readable data-storage medium comprising a data-storage material in which the structure coordinates of an LBD according to Claim 1 are stored.
 - 9. A computer-readable data-storage medium comprising a data-storage material in which the structure coordinates of an LBD according to Claim 1 are stored in a form which makes it possible to generate a three-dimensional image of an LBD according to Claim 1 on a computer screen.
 - 10. A method for generating protein models of USP-LBDs, comprising the step of preparing by computer-aided generation a three-dimensional image of an LBD according to Claim 1.
- 25 11. A method for generating protein models of USP-LBDs in an agonistic conformation comprising the step of preparing by computer-aided generation a three-dimensional image of an LBD according to Claim 1 in an agonistic conformation.
- 30 12. A method for generating protein models of nuclear receptors with homologies to USP-LBDs, comprising the step of preparing by computer-aided

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generation a three-dimensional image of an LBD according to Claim 1 with a mutated amino acid sequence.

- 13. A method for generating protein models of nuclear receptors with homologies to USP-LBDs, in an agonistic conformation, comprising the step of preparing by computer-aided generation a three-dimensional image of an LBD according to Claim 1 with a mutated amino acid sequence in an agonistic conformation.
- 10 14. A method of finding USP ligands, comprising the steps of:
 - (a) preparing by computer-aided generation a three-dimensional image of an LBD according to Claim 1, and
 - (b) performing computer-aided (virtual) screening of databases which contain structural data of chemical compounds for those structures which are capable of undergoing specific interactions with an LBD according to Claim 1.
 - 15. A method of finding USP ligands, comprising the steps of:
 - (a) preparing by computer-aided generation a three-dimensional image of an LBD according to Claim 1, and
 - (b) performing computer-aided modelling of chemical compounds with structures which are capable of undergoing specific interactions with an LBD according to Claim 1.
- 25 16. A method of finding USP-LBD ligands in an agonistic conformation, comprising the steps of:
 - (a) preparing by computer-aided generation a three-dimensional image of an LBD according to Claim 1 in an agonistic conformation, and
 - (b) performing computer-aided (virtual) screening of databases which contain structural data of chemical compounds for those structures which are capable of undergoing specific interactions with an LBD in an agonistic conformation.

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- 17. A method of finding USP-LBD ligands in an agonistic conformation, comprising the steps of:
 - (a) preparing by computer-aided generation a three-dimensional image of an LBD according to Claim 1 in an agonistic conformation, and
 - (b) performing computer-aided modelling of chemical compounds with structures which are capable of undergoing specific interactions with an LBD in an agonistic conformation.
- 10 18. A method of finding active compounds for crop protection, in particular chemical compounds which, owing to binding to an LBD according to Claim 1, bring about the activation or inhibition of USP, comprising the steps of:
 - preparing by computer-aided generation a three-dimensional image (a) of an LBD according to Claim 1,
 - performing computer-aided (virtual) screening of databases which (b) contain structural data of chemical compounds for those structures which are capable of undergoing specific interactions with an LBD according to Claim 1,
- 20 (c) synthesizing the compound(s) identified as ligands, and
 - (d) detecting the bioactivity of the compound synthesized in step (c) by transactivation assays, displacement assays or bioassays.
- 19. A method of finding active compounds for crop protection, in particular 25 chemical compounds which, owing to binding to an LBD according to Claim 1 in an agonistic conformation, bring about the activation or inhibition of USP, comprising the steps of:
 - preparing by computer-aided generation a three-dimensional image (a) of an LBD according to Claim 1 in an agonistic conformation,
- 30 (b) performing computer-aided (virtual) screening of databases which contain structural data of chemical compounds for those structures

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which are capable of undergoing specific interactions with an LBD in an agonistic conformation,

- (c) synthesizing the compound(s) identified as ligands, and
- (d) detecting the bioactivity of the compound synthesized in step (c) by transactivation assays, displacement assays or bioassays.
- 20. A method of finding effectors for systems for the inducible expression of target genes by means of USP, comprising the steps of:
 - (a) preparing by computer-aided generation a three-dimensional image of an LBD according to Claim 1,
 - (b) performing computer-aided (virtual) screening of databases which contain structural data of chemical compounds for those structures which are capable of undergoing specific interactions with an LBD according to Claim 1,
 - (c) synthesizing the compound(s) identified as ligands,
 - (d) applying a compound synthesized in step (c) to host cells or host organisms comprising a USP-based expression system, and
 - (e) detecting an induction or inhibition of the expression system.:
- 20 21. A method of finding active compounds for crop protection, in particular chemical compounds which, owing to binding to an LBD according to Claim 1, bring about the activation or inhibition of USP, comprising the steps of:
 - (a) preparing by computer-aided generation a three-dimensional image of an LBD according to Claim 1,
 - (b) performing computer-aided modelling of chemical compounds with structures which are capable of undergoing specific interactions with an LBD according to Claim 1,
 - (c) synthesizing the compound(s) identified as ligands, and
- detecting the bioactivity of the compound synthesized in step (c) by transactivation assays, displacement assays or bioassays.

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- 22. A method of finding active compounds for crop protection, in particular chemical compounds which, owing to binding to an LBD according to Claim 1 in an agonistic conformation, bring about the activation or inhibition of USP, comprising the steps of:
 - preparing by computer-aided generation a three-dimensional image (a) of an LBD according to Claim 1 in an agonistic conformation, and
 - (b) performing computer-aided modelling of chemical compounds with structures which are capable of undergoing specific interactions with an LBD in an agonistic conformation.
 - synthesizing the compound(s) identified as ligands, and (c)
 - detecting the bioactivity of the compound synthesized in step (c) by (d) transactivation assays, displacement assays or bioassays.
- 23. A method of finding effectors for systems for the inducible expression of target genes by means of USP, comprising the steps of:
 - preparing by computer-aided generation a three-dimensional image (a) of an LBD according to Claim 1,
 - performing computer-aided modelling of chemical compounds (b) with structures which are capable of undergoing specific interactions with an LBD according to Claim 1,
 - (c) synthesizing the compound(s) identified as ligands,
 - applying a compound synthesized in step (c) to host cells or host (d) organisms comprising a USP-based expression system, and
 - detecting an induction or inhibition of the expression system. (e)